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COLLISIONAL PROCESSES OF HYDROCARBONS
IN HYDROGEN PLASMAS

By

A.B. Ehrhardt and W.D. Langer

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COLLISIONAL PROCESSES OF HYDROCARBONS IN HYDROGEN PLASMAS

A.B. Ehrhardt and W.D. Langer

Plasma Physics Laboratory, Princeton University

Princeton, NJ 08544

ABSTRACT

We have investigated the reactions of methane and its derivatives with hydrogen plasmas for use in modelling carbon and hydrocarbon transport in hydrogen plasmas. We provide quantitative information over the temperature range from 0.1 eV to 2 keV for the most significant reactions of methane and methane fragments with electrons and protons. We review the properties of each reaction, present graphs of the cross section and reaction rate coefficient, and give analytical fits for σ and $\langle\sigma v\rangle$.

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1. INTRODUCTION

The transport and recycling of carbon and hydrocarbons is of increasing importance in studies of tokamak plasmas because limiters are made of graphite and the interaction of ions and energetic neutrals from the plasma can cause the limiters to release carbon and hydrocarbons (principally, methane and acetylene). Also, carbon films have been suggested as a wall coating in tokamaks to control and reduce impurity release of high-Z wall materials (cf. the review of carbonization in tokamaks by Winter 1987). To model the particle and energy transport and power loss in plasmas due to carbon, many collisional processes need to be known over a wide range of plasma conditions, especially at the plasma edge where temperatures are low (<1 keV). Furthermore, data of this type are useful for studies of plasma processing of materials, such as semiconductors. The two earlier surveys of Langer [1982] and de Heer [1981] are based on work done before 1980 and so it is timely to update what is known about methane reactions.

Our survey provides a data base for atomic and molecular collisions for carbon and methane with hydrogen plasmas with temperatures between 0.1 eV and 2 keV, and electron and ion densities less than about $5 \times 10^{14} \text{ cm}^{-3}$. We present descriptions of the reactions and graphs of the cross sections and reaction rate coefficients for all types of inelastic processes between hydrocarbons and the electrons and ions in the plasma. We also include an estimate of the energetics of the reaction (energy loss or gain in the reaction, energy distribution of reaction products, etc.). Finally, we give analytic fits to the cross sections and reaction rate coefficients. The survey is in a form designed for use in modelling and is not intended as a treatise on the details of the reaction dynamics.

1.1. Organization of Information

Here, we describe the form for presentation of the data and the units and notation. The units for the more common quantities used throughout the text are:

E: impact energy, in the laboratory reference system, in eV, unless otherwise stated;

σ : cross section in cm^2 ;

$\langle\sigma v\rangle$: reaction rate coefficient in cm^3/s , the average being taken over a Maxwellian distribution at temperature T (eV) of the charged particle.

For each individual reaction we give the following information in order of presentation:

- (1) symbolic notation,
- (2) energy loss or gain,
- (3) the method (experimental, theoretical, or semiempirical), by which the cross section has been obtained in various energy regions with reference to the corresponding data source,
- (4) energetics of the reaction products (when applicable),
- (5) comments on the reaction and/or the procedures applied to determine the cross sections,
- (6) a graphical representation of the cross section σ as a function of energy E (represented by a dashed curve with the scale on the right-hand side) and the corresponding reaction rate coefficient $\langle\sigma v\rangle$ as a function of temperature T (given by a solid line with the scale on the left side),
- (7) in the case of reactions between heavy particles, the target particle's energy (velocity) can be important, and the figures show the reaction rate coefficients as a function of plasma temperature at several energies of the target particle,

- (8) in the case of reactions between plasma electrons and heavier particles, the heavy particle's energy is taken to be zero and only the temperature dependence is plotted.

1.2 Sources and Criteria for the Atomic Physics Data

The main source of information for the cross sections were the current journal literature and previous compilations. Where the cross section data do not cover the entire energy range considered here, we have extended the range by employing appropriate interpolation or extrapolation procedures based either on theoretical models or on a reasonable extension or scaling of the experimental data.

1.3 Accuracy of Data

In general, the accuracy for the measured cross section data for processes involving ground state species is $\pm 50\%$ or better. However, there are many reactions for which no measurements exist where we had to be guided by theoretical considerations or deduce the expected behavior from other measurements. In these cases, the user should be well aware of the possibility that the cross sections could be seriously in error.

1.4 Calculation of Reaction Rate Coefficients

The calculation of reaction rate coefficients was made using SIGMAV, an updated version of the program MODIFY developed for the survey of hydrogen reactions by Janev et al. (1987). Here, we review a few key points of their method for calculating $\langle \sigma v \rangle$.

The Maxwellian-averaged reaction rate coefficients for a particle of mass m and fixed energy $E = mv^2/2$ incident on a Maxwellian distribution of

particles of mass M and temperature $T = Mu^2/2$ is, for the heavy-particle reactions,

$$\langle\sigma v\rangle = \frac{1}{\pi^{1/2} u^3} \int_{v_{th}}^{\infty} v_r^2 dv_r \sigma(E_r) \{ \exp[-(v_r - v)^2/u^2] - \exp[-(v_r + v)^2/u^2] \},$$

and for the electron reactions,

$$\langle\sigma v\rangle = \frac{4}{\pi^{1/2} u^3} \int_{v_{th}}^{\infty} v_r^3 dv_r \sigma(E_r) \exp(-v_r^2/u^2),$$

where $v_r = |\vec{v} - \vec{u}|$ is the relative (collision) velocity, with $E_r = m_r v_r^2/2$, $m_r = mM/(m + M)$ being the reduced mass of colliding particles, and v_{th} the value of v_r at threshold, $E_r = E_{th}$.

We calculated the cross sections used in the plots, in the numerical tables, and in the integrals for the reaction rate coefficients, including both interpolations and extrapolations of the data, by the procedures described in Janev et al. (1987).

1.5 Numerical Fits to σ and $\langle\sigma v\rangle$

Numerical fits were derived for σ and $\langle\sigma v\rangle$ using the same approach described in Janev et al. (1987). We made polynomial fits for $\ln \sigma$ in terms of $\ln E$,

$$\ln \sigma = \sum_{n=0}^N a_n (\ln E)^n.$$

For the electron reactions, $\langle\sigma v\rangle$ is essentially independent of E within the range of energies considered here, and we evaluated $\langle\sigma v\rangle$ only in terms of T :

$$\ln \langle \sigma v \rangle = \sum_{n=0}^N b_n (\ln T)^n .$$

A more useful fit for the heavy-particle reactions is a double polynomial fit in both E and T:

$$\ln \langle \sigma v \rangle = \sum_{n=0}^N \sum_{m=0}^M a_{mn} (\ln E)^n (\ln T)^m .$$

An error is given for each fit as an indication of the quality of the fit. The error is defined as

$$\frac{1}{N} \sum_{i=1}^N (\ln x_i - \ln x_{\text{fit},i})^2 ,$$

where N is the number of points fit, and x is σ or $\langle \sigma v \rangle$. An error of 10^{-4} or less is a good fit very close to the actual values and, most likely, well within the error in the data.

Under some conditions an empirical modification of the Bethe-Born formula can be useful in fitting σ (see Lotz 1967, and Janev et al. 1987). We provide such fits, as described in Sec. 4.1, but, in general, these were not as good as the polynomial fits.

1.6 Example of Use of Fits

As an example of the use of the tables of fits for cross sections and reaction rate coefficients consider the calculation of $\langle \sigma v \rangle$ for reaction 2.1, $e + CH_4 \rightarrow CH_4^+ + e + e'$, at $T = 10$ eV. The nine fitting coefficients are listed immediately below the reaction number and label in the Table. At the bottom, we give the minimum temperature, $T_{\min} = 1.58e00$ eV, for which the fit is valid and the corresponding value of the reaction rate coefficient,

$\langle\sigma v\rangle(T_{\min}) = 3.52e-12 \text{ cm}^3/\text{s}$. The maximum temperature at which the fit is valid is 2000 eV, unless otherwise noted. We also list the maximum value of the reaction rate coefficient over the valid range of the fit, in this case, $\langle\sigma v\rangle_{\max} = 1.04e-07 \text{ cm}^3/\text{s}$. The reaction rate coefficient is computed as follows:

$$\ln \langle\sigma v\rangle = \sum_{n=0}^8 b_n (\ln T)^n.$$

At $T = 10 \text{ eV}$ using the coefficients for reaction 2.1 in Sec. 4.2 (these are truncated at six digits since this number is sufficient for a nearly perfect fit), we have

$$\begin{aligned}\ln \langle\sigma v\rangle &= -3.13027e+01 + 1.29616e+01(2.30259) \\ &\quad -5.50027e+00(2.30259)^2 + 1.46875e+00(2.30259)^3 \\ &\quad -2.51540e-01(2.30259)^4 + 2.71002e-02(2.30259)^5 \\ &\quad -1.78660e-03(2.30259)^6 + 6.60557e-05(2.30259)^7 \\ &\quad -1.05104e-06(2.30259)^8\end{aligned}$$

$$\ln \langle\sigma v\rangle = -18.2499.$$

Thus,

$$\langle\sigma v\rangle = 1.18619e-08 \text{ cm}^3/\text{s}.$$

Finally, the error of the fit is given, $3.54e-06$, which for this reaction means that the fit is indistinguishable from the calculated curve (see the figure after reaction 2.1).

1.7 Acknowledgements

We would like to thank Dr. Ken Evans, Jr. of Argonne National Laboratory for the use of his program MODIFY to process the cross section data, calculate the reaction rate coefficients, provide plots, and compute the fits. His help was invaluable in understanding and using the program. The program SIGMAV used to process the methane and carbon reactions in this report is our updated version of MODIFY with enhanced graphics.

Much of the impetus for this work derived from its planned application to 3-D neutral particle transport in plasma devices, and we gratefully acknowledge the contributions of Dr. Daniel Heifetz, of Princeton Plasma Physics Laboratory during the process of adding to the DEGAS Neutral Gas Transport Code the capacity to follow methane and carbon.

We also appreciate the continuing assistance and patience of Ms. Betty Carey and Ms. Ceil O'Brien through the many drafts of this document.

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LIST OF SYMBOLS AND ABREVIATIONS

E	- impact energy
E_{th}	- threshold energy
$\Delta E_i^{(-)}$	- kinetic energy <u>loss</u> of particle i in a reaction
$\Delta E_i^{(+)}$	- kinetic energy <u>gain</u> of particle i in a reaction
$\langle A \rangle_\gamma$	- quantity A averaged over a finite interval of the parameter γ , where γ can be continuous or discrete. For example, FC would denote Franck-Condon interval, and v vibrational levels.
T	- Maxwellian temperature
v	- collisional velocity or vibrational quantum number
σ_j	- cross section of reaction j
σ_j^B	- cross section in the first Born approximation
σ_{se}	- semiempirical cross section
σ_{exp}	- experimental cross section
σ_{ion}	- ionization cross section
σ_{di}	- dissociative ionization cross section
σ_{dr}	- dissociative recombination cross section
σ_i^{tot}	- total cross section of reaction type i
σ_{cx}	- charge exchange cross section
σ_{ext}	- empirical extrapolation of cross section

LIST OF REACTIONS

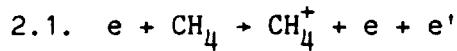
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2. ELECTRON IMPACT COLLISION PROCESSES

2. ELECTRON IMPACT COLLISION PROCESSES



$$E_{\text{th}} = 12.6 \text{ eV}$$

Cross Section:

$$E = E_{\text{th}} - 2000 \text{ eV} \quad \sigma_{\text{ion}} = \sigma_{\text{exp}}$$

References: Chatham et al. (1984)

Rapp and Englander-Golden (1965)

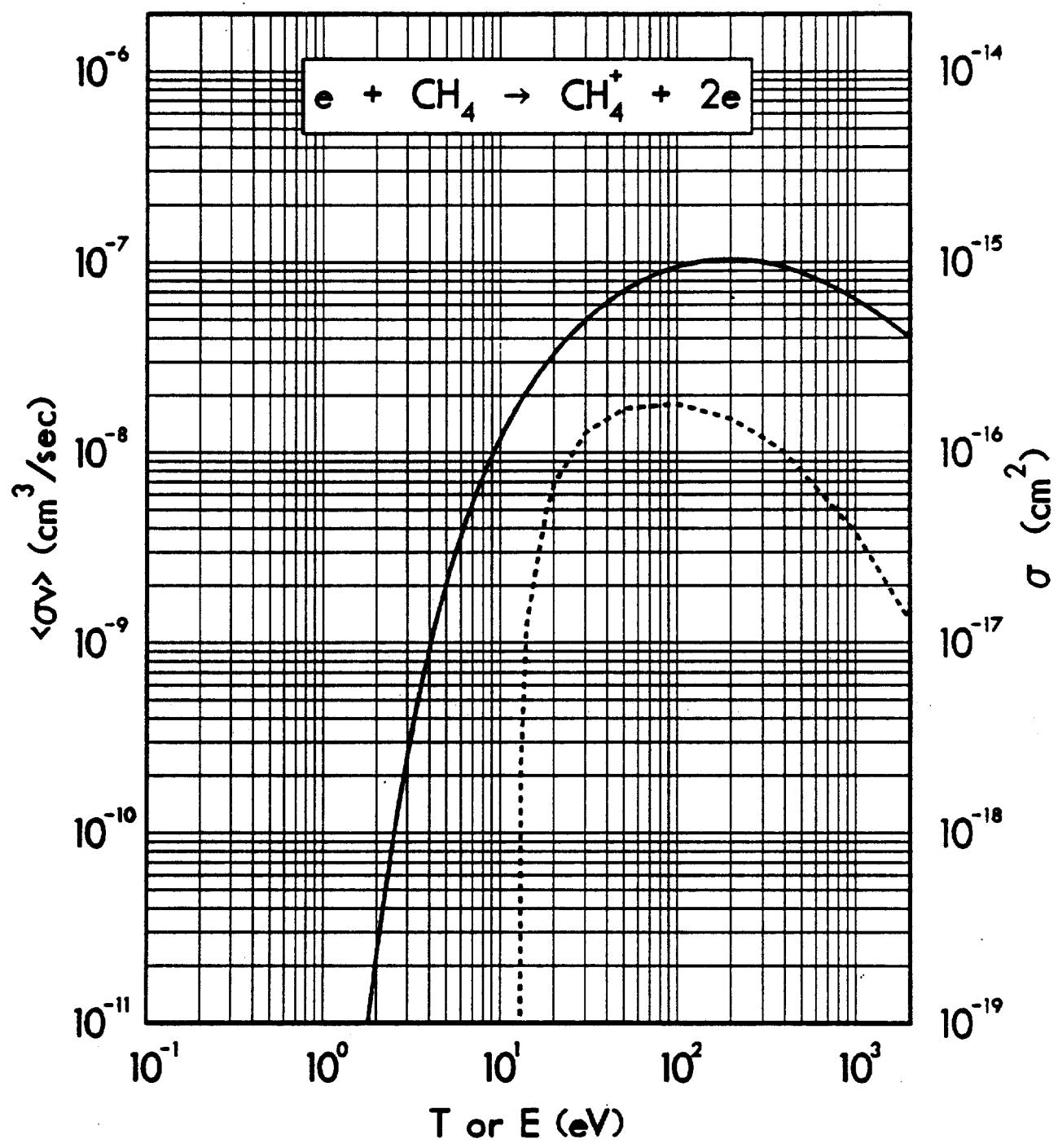
Adamczyk et al. (1966)

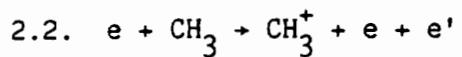
Energetics:

$$\Delta E_{e'}^{(+)} = 2 \text{ eV} \quad \Delta E_{e'}^{(-)} = 15 \text{ eV}$$

Comments:

- (1) A semiempirical cross section fit by Tan and Wu (1977) is in good agreement with the experimental data.
- (2) We set the energy loss to be typically 15 eV consistent with the Franck-Condon overlap and the large increase in σ at 15 eV (cf. Mather 1980; Marmet and Binette 1978).





$$E_{th} = 12.6 \text{ eV}$$

Cross Section:

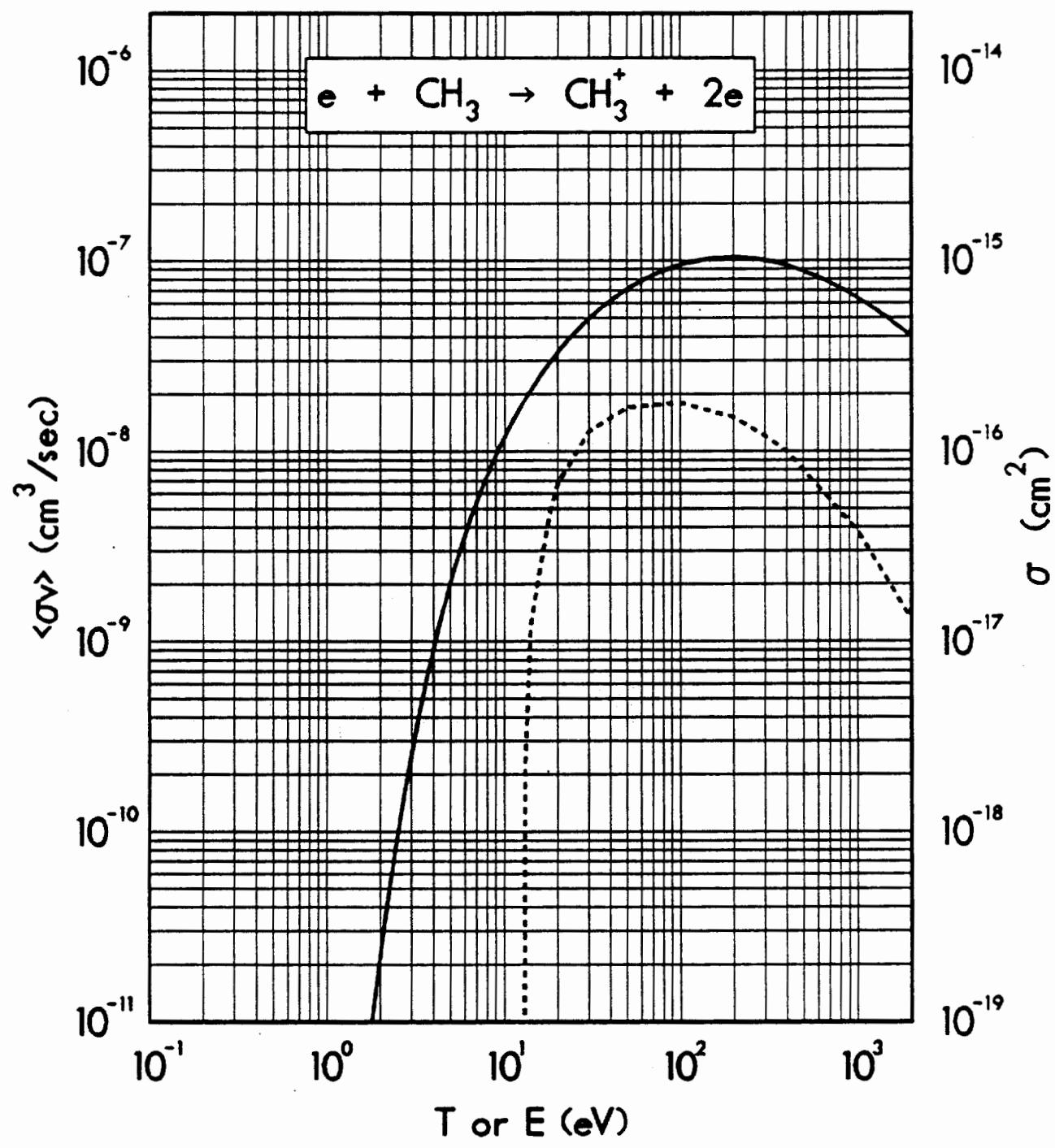
$$\begin{aligned} E &= E_{\min} - 200 \text{ eV} & \sigma_{\text{ion}} &= \sigma_{\text{exp}}(\text{CD}_3) \\ &= 200 - 2000 \text{ eV} & \sigma_{\text{ion}} &= \sigma_{\text{exp}}(\text{CH}_4) \end{aligned}$$

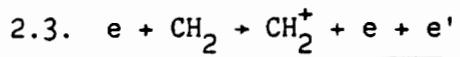
References: Baiocchi et al. (1984)

Energetics:

$$\Delta E_e^{(-)} = 15 \text{ eV} \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

Comments: Baiocchi, Wetzel, and Freund (1984) measured ionization cross sections for CD_3 up to 200 eV and found values very close to those measured for CH_4 above 15 eV. Hence, we have adopted the CH_4 cross section values for CH_3 below 15 eV, especially since vibrational excitation and the presence of metastables may have affected the low energy results for CD_3 . The error in the measurements, in any case, is estimated to be $\pm 30\%$.





$$E_{\min} = 12.6 \text{ eV}$$

Cross Section:

$$E = E_{\min} - 200 \text{ eV} \quad \sigma_{\text{ion}} = \sigma_{\text{exp}}(CD_2)$$

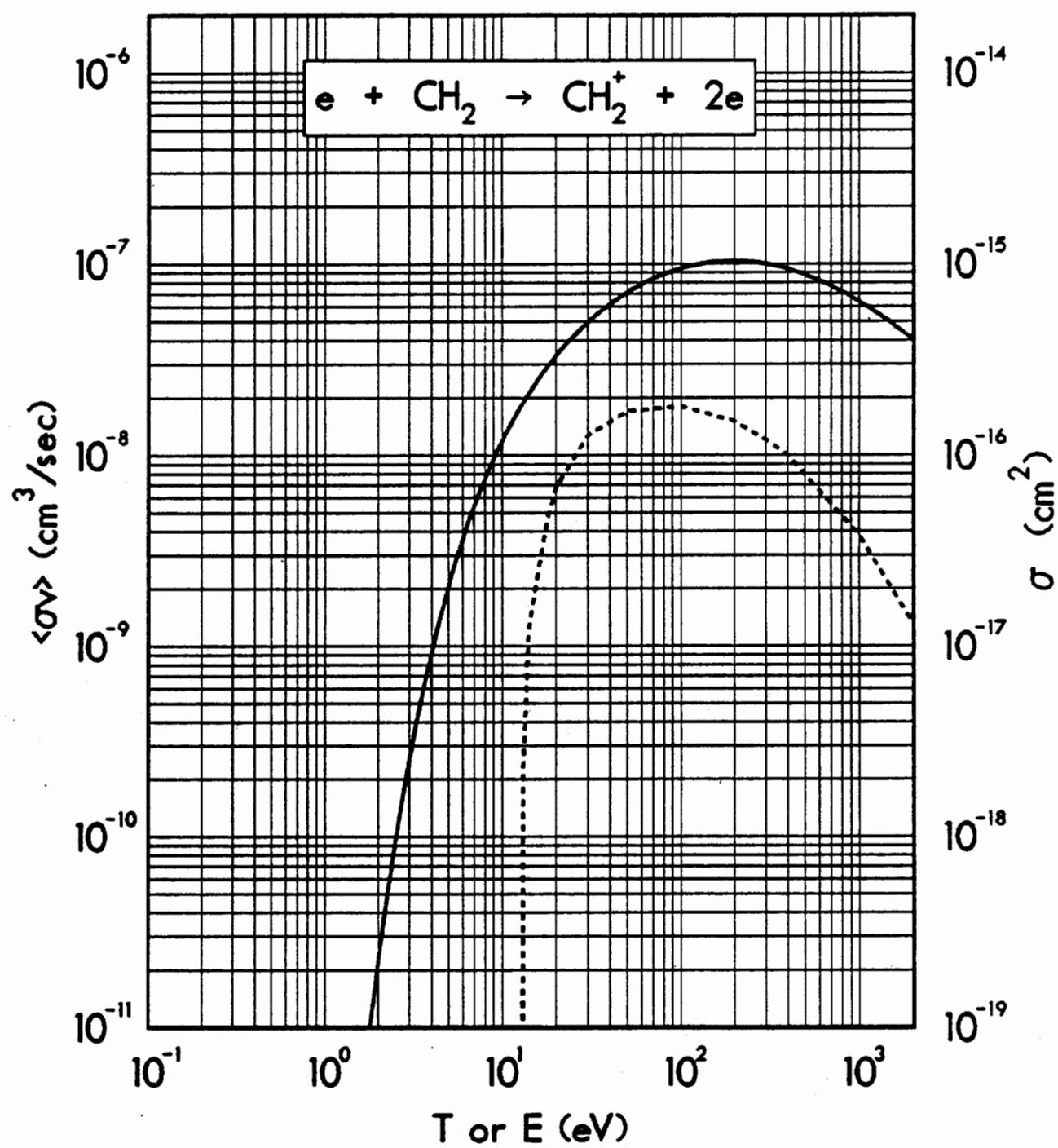
$$E = 200 - 2000 \text{ eV} \quad \sigma_{\text{ion}} = \sigma_{\text{exp}}(CH_4)$$

References: Baiocchi et al. (1984)

Energetics:

$$\Delta E_e^{(-)} = 15 \text{ eV} \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

Comments: The measured ionization cross section for CD_2 (Baiocchi et al.) is very close to those for CD_3 and CH_4 over the energy range 15 to 200 eV, being only about 15% higher than those of CD_3 above 100 eV. Therefore, we use the CH_4 results of reaction 2.1 below 15 eV and above 200 eV. See additional comments in reaction 2.2.





$$E_{\min} = 12.6 \text{ eV}$$

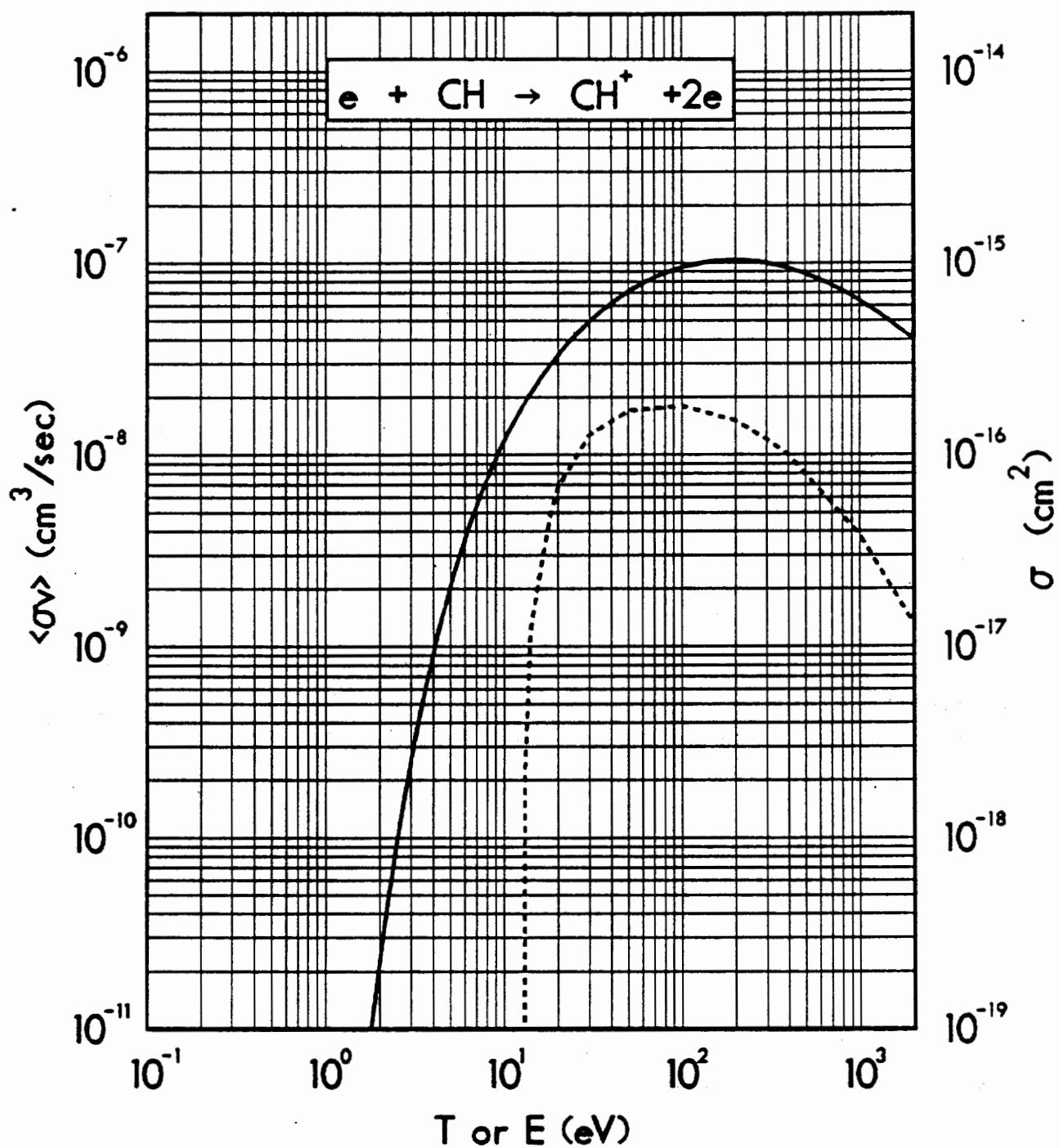
Cross Section:

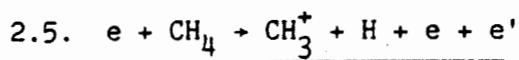
$$E = E_{\min} - 2000 \text{ eV} \quad \sigma_{\text{ion}}(\text{CH}) = \sigma_{\text{exp}}(\text{CH}_4)$$

Energetics:

$$\Delta E_e^{(-)} = 15 \text{ eV} \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

Comments: In light of the similar cross sections for ionizing CH_4 , CD_3 , and CD_2 over the energy range 15-200 eV, we have adopted the CH_4 experimental results for CH.





$$E_{\text{th}} = 14.3 \text{ eV}$$

Cross Section:

$$E = E_{\text{th}} - 2000 \text{ eV} \quad \sigma_{\text{di}} = \sigma_{\text{exp}}$$

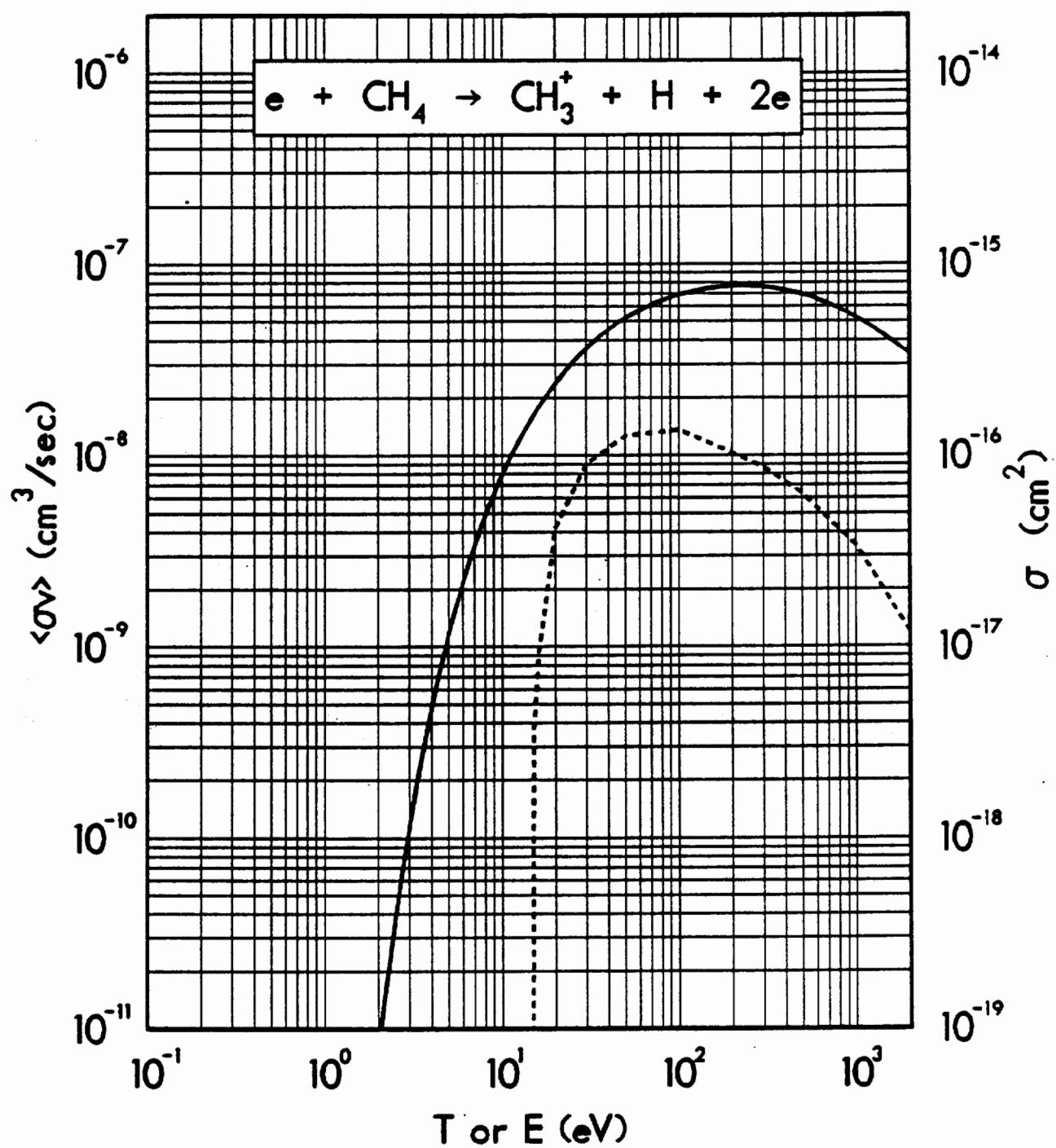
References: Chatham et al. (1984), Adamczyk et al. (1966)

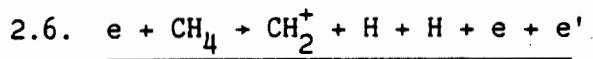
Energetics:

$$\Delta E_e^{(-)} = 20 \text{ eV} \quad \Delta E_e^{(+)} = 2 \text{ eV}$$

$$\Delta E_H^{(+)} \approx 3 \text{ eV} \quad \Delta E_{\text{CH}_3^+}^{(+)} \approx 0.3 \text{ eV}$$

Comments: The electron energy loss (gain) is estimated using the same criterion as in reaction 2.1. A portion of the energy transferred to CH_4 appears as kinetic energy of the heavier fragments. The excited states of CH_4 (Marmet and Binette 1978) lie between 18 and 22 eV (Schiavone, Tarr, and Freund 1979) in the Franck-Condon region which suggests that about several eV goes into kinetic energy of the fragments (mostly into H). Laboratory measurements support this suggestion. At electron energies less than 40 eV, the average kinetic energy is about 2.5 eV and increases to 4 eV above an electron energy of 50 eV (Ito et al. 1977); here, we adopt 3 eV as a typical value.





$$E_{th} = 15.1 \text{ eV}$$

Cross Sections:

$$E = E_{th} - 2000 \text{ eV} \quad \sigma_{di} = \sigma_{exp}$$

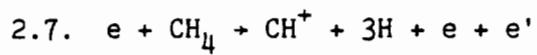
References: Chatham et al. (1984); Adamczyk et al. (1966)

Energetics:

$$\Delta E_e^{(-)} = 21 \text{ eV} \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

$$\Delta E_H^{(+)} \approx 1.5 \text{ eV per H} \quad \Delta E_{CH_2^+}^{(+)} \approx 0.3 \text{ eV}$$

Comments: Reaction rate coefficients are not calculated as the cross section comprises less than 7% of the total ionization cross section. The energetics are similar to those in reaction 2.5 with the hydrogen kinetic energy divided equally between the two hydrogens.



$$E_{th} = 22.2 \text{ eV}$$

Cross Section:

$$E = E_{th} - 2000 \text{ eV} \quad \sigma_{di} = \sigma_{exp}$$

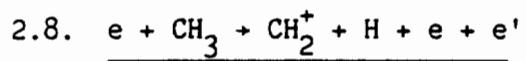
References: Chatham et al. (1984), Adamczyk et al. (1966)

Energetics:

$$\Delta E_e^{(-)} = 28 \text{ eV} \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

$$\Delta E_H^{(+)} \approx 1 \text{ eV} \quad \Delta E_{CH^+}^{(+)} \approx 0.3 \text{ eV}$$

Comment: This term contributes less than 2% to the ionization of CH_4 , and its reaction rate coefficient is not calculated. Energetics are similar to reaction 2.5 with the hydrogen kinetic energy divided equally among the three hydrogens.



$$E_{\min} = 15.0 \text{ eV}$$

Cross Sections:

$$E = E_{\min} - 200 \text{ eV} \quad \sigma_{di} = \sigma_{exp} (\text{CD}_3)$$

$$E = 200 - 2000 \text{ eV} \quad \sigma_{di} = \sigma_{se}$$

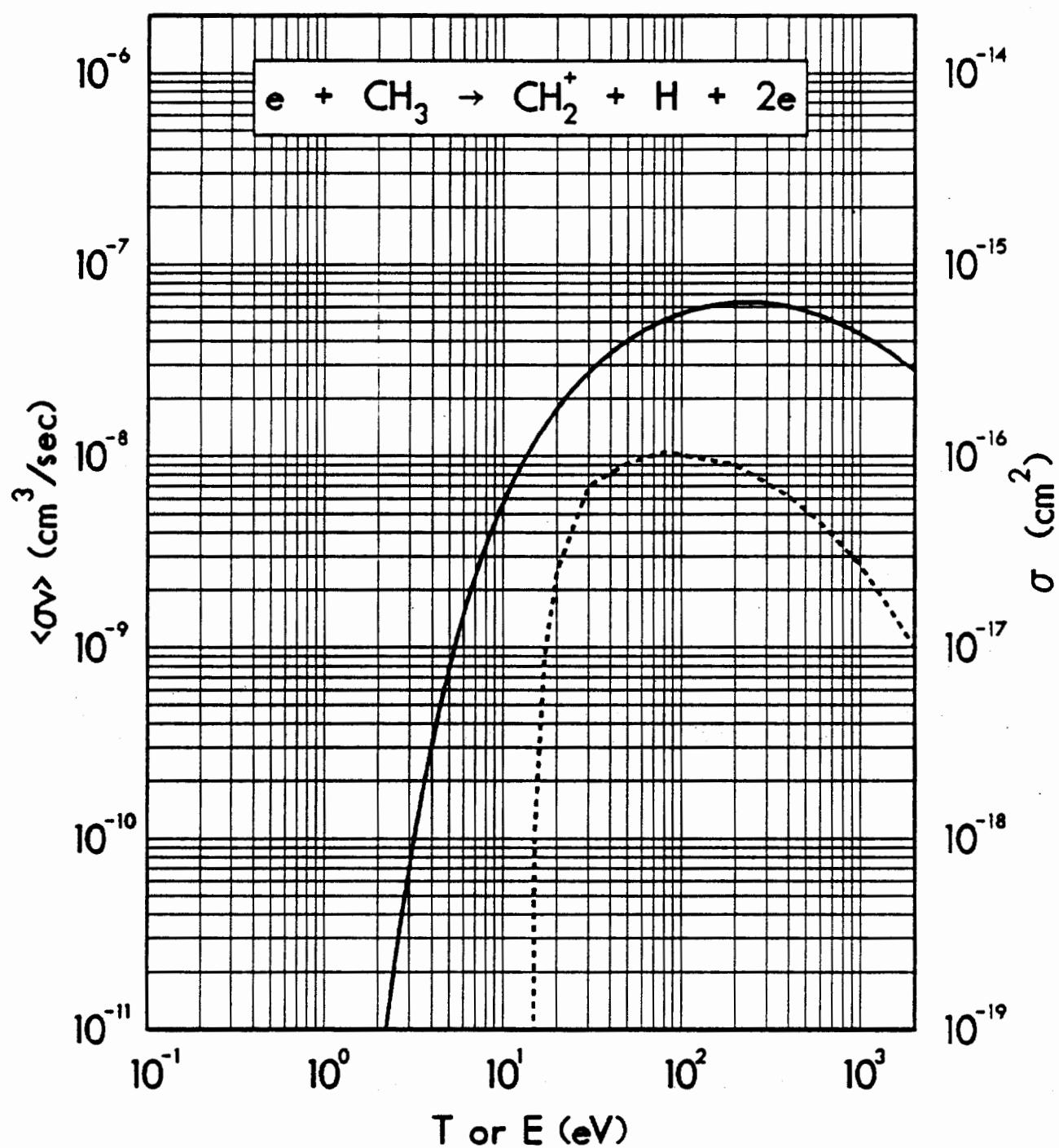
References: Baiocchi, Wetzel, and Freund (1984)

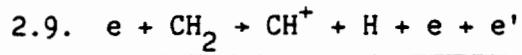
Energetics:

$$\Delta E_e^{(-)} = 20 \text{ eV} \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

$$\Delta E_H^{(+)} \approx 3 \text{ eV} \quad \Delta E_{\text{CH}_2^+}^{(+)} \approx 0.3 \text{ eV}$$

Comments: The cross section values for CH_3 are assumed to be the same as those for CD_3 , the species studied by Baiocchi et al. The semiempirical extrapolation for CH_3 is based on the data for CH_4 dissociative ionization because up to 200 eV σ_{di} for CD_3 scales reasonably well with σ_{ion} (see Fig. 2, Baiocchi et al.). The energetics of the heavy particles are evaluated on the same basis as those of reaction 2.5.





$$E_{\min} = 17.9 \text{ eV}$$

Cross Sections:

$$E = E_{\min} - 200 \text{ eV} \quad \sigma_{di} = \sigma_{exp}(\text{CD}_2)$$

$$= 200 - 2000 \text{ eV} \quad \sigma_{di} = \sigma_{se}$$

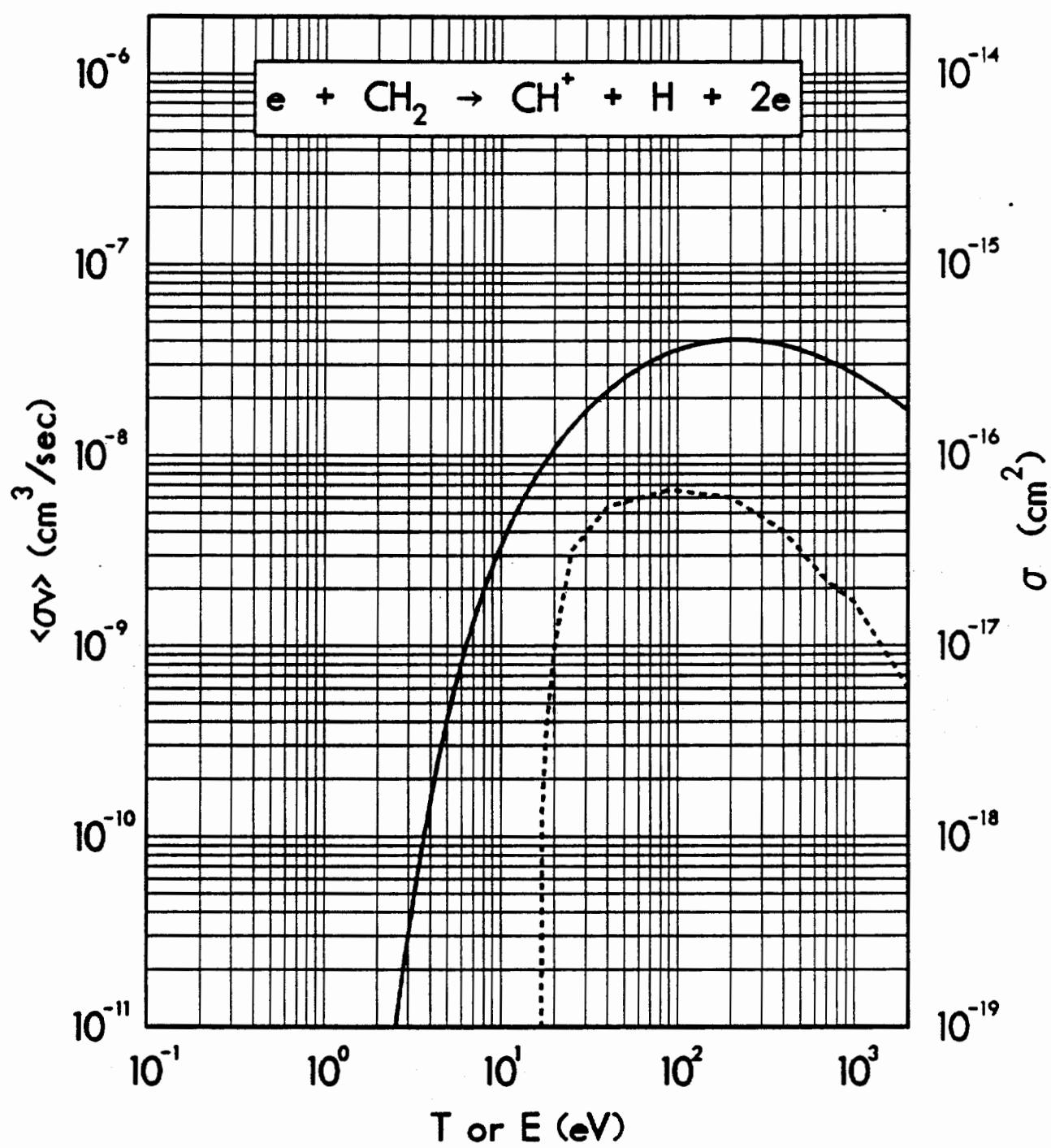
References: Baiocchi, Wetzel, and Freund (1984).

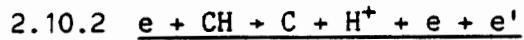
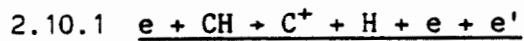
Energetics:

$$\Delta E_e^{(-)} = 23 \text{ eV}, \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

$$\Delta E_H^{(+)} \approx 3 \text{ eV} \quad \Delta E_{\text{CH}^+}^{(+)} \approx 0.3 \text{ eV}$$

Comments: See comments for reaction 2.8.





$$\langle E_{\min} \rangle = 17.0 \text{ eV}$$

Cross Section:

$$E = E_{\min} - 2000 \text{ eV} \quad \sigma_{di}(\text{total}) = \sigma_{se}$$

$$2.10.1 \quad \sigma_{di} (+ C^+ + H + 2e) = \alpha \sigma_{di}^{\text{tot}} = 0.5 \sigma_{di}^{\text{tot}}$$

$$2.10.2 \quad \sigma_{di} (+ C + H^+ + 2e) = (1 - \alpha) \sigma_{di}^{\text{tot}} = 0.5 \sigma_{di}^{\text{tot}}$$

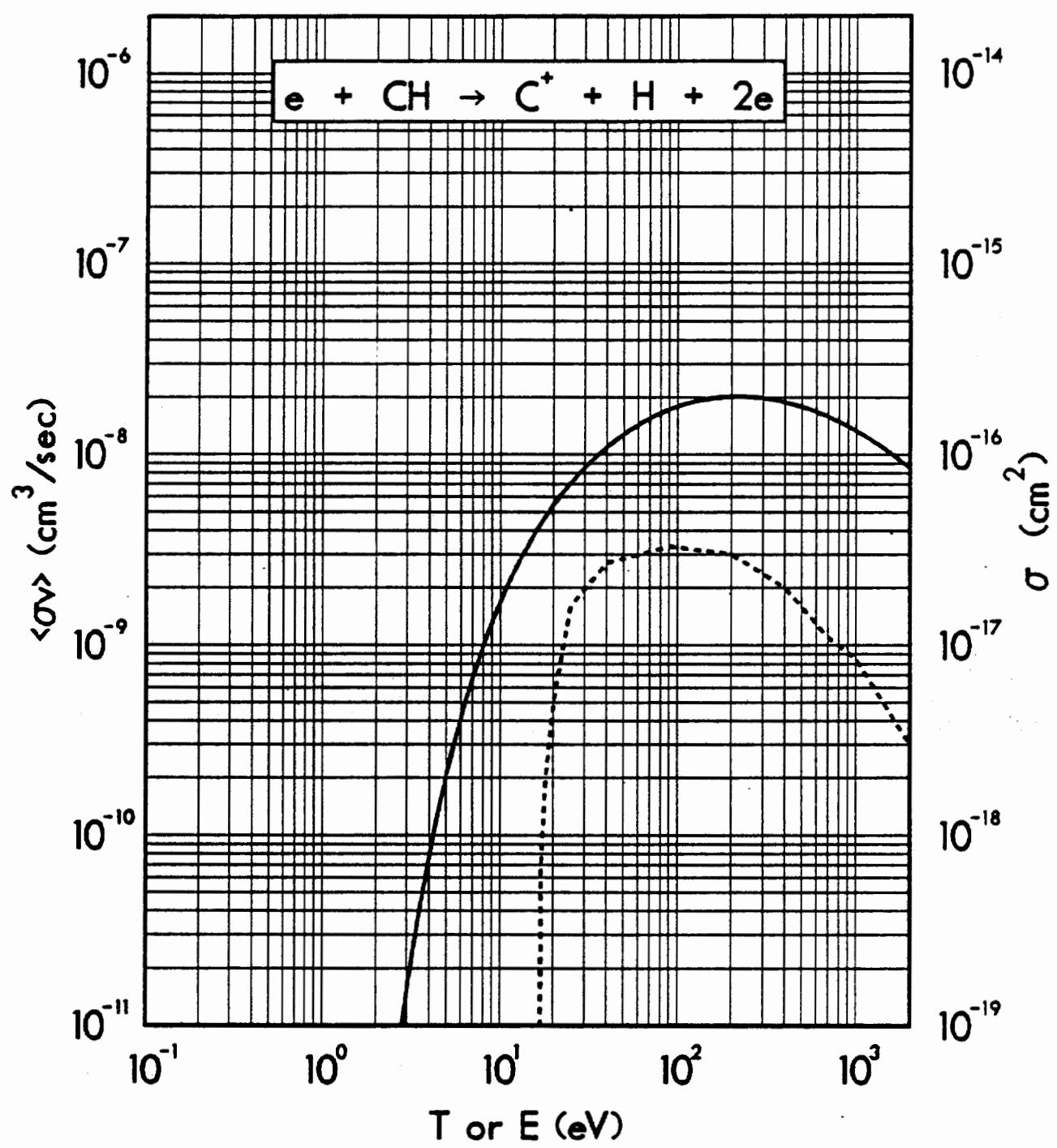
Energetics:

$$\Delta E_e^{(-)} = 22 \text{ eV} \quad \Delta E_{e'}^{(+)} = 2 \text{ eV}$$

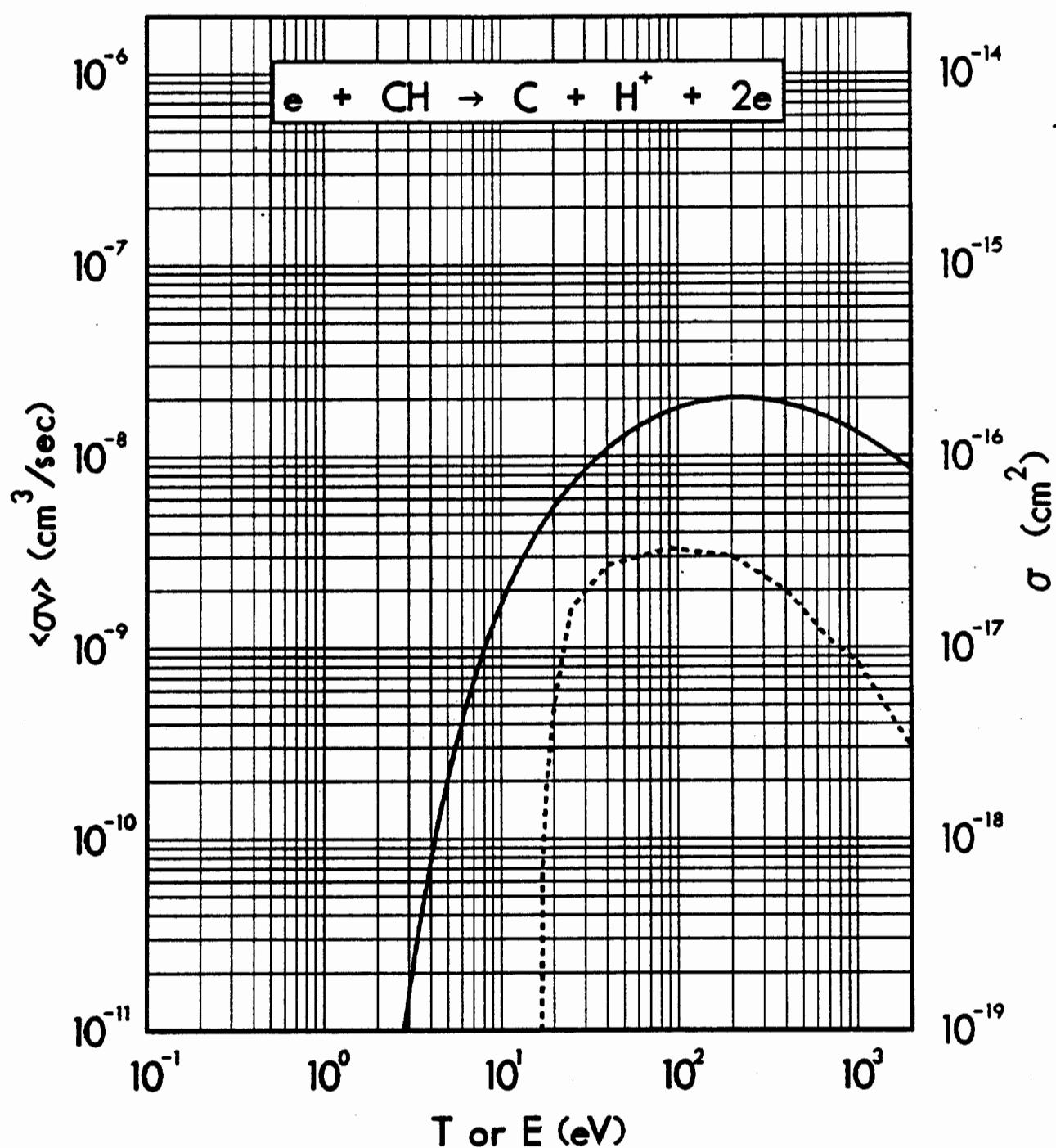
$$\Delta E_{(C^+ \text{ or } C)}^{(+)} \approx 0.3 \text{ eV} \quad \Delta E_{(H \text{ or } H^+)}^{(+)} \approx 3 \text{ eV}$$

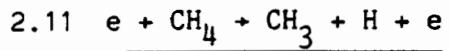
Comments:

- (1) We assume that the total dissociative ionization cross section for CH is half that for CH_2 (see reaction 2.8) as indicated by the experimental data for CH_4 , CD_3 , and CD_2 . σ_{di} should scale like n , where n equals the number of hydrogens in CH_n .
- (2) The branching ratio, α , is taken to be about one-half because there appear to be a comparable number of accessible states for both channels within the Franck-Condon region (see potential energy curves in Lorquet et al. 1971). The energetics are evaluated as in reaction 2.5.



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$$E_{\min} = 10 \text{ eV}$$

Cross Section:

$$10 < E < 500 \text{ eV}$$

$$\sigma_d = \sigma_{\text{exp}} = \sigma_{d+di}^{\text{tot}} - \sigma_{di}^{\text{tot}}$$

$$E > 500 \text{ eV}$$

$$\sigma_d = \sigma_{\text{se}}$$

Reference: Winters (1975)

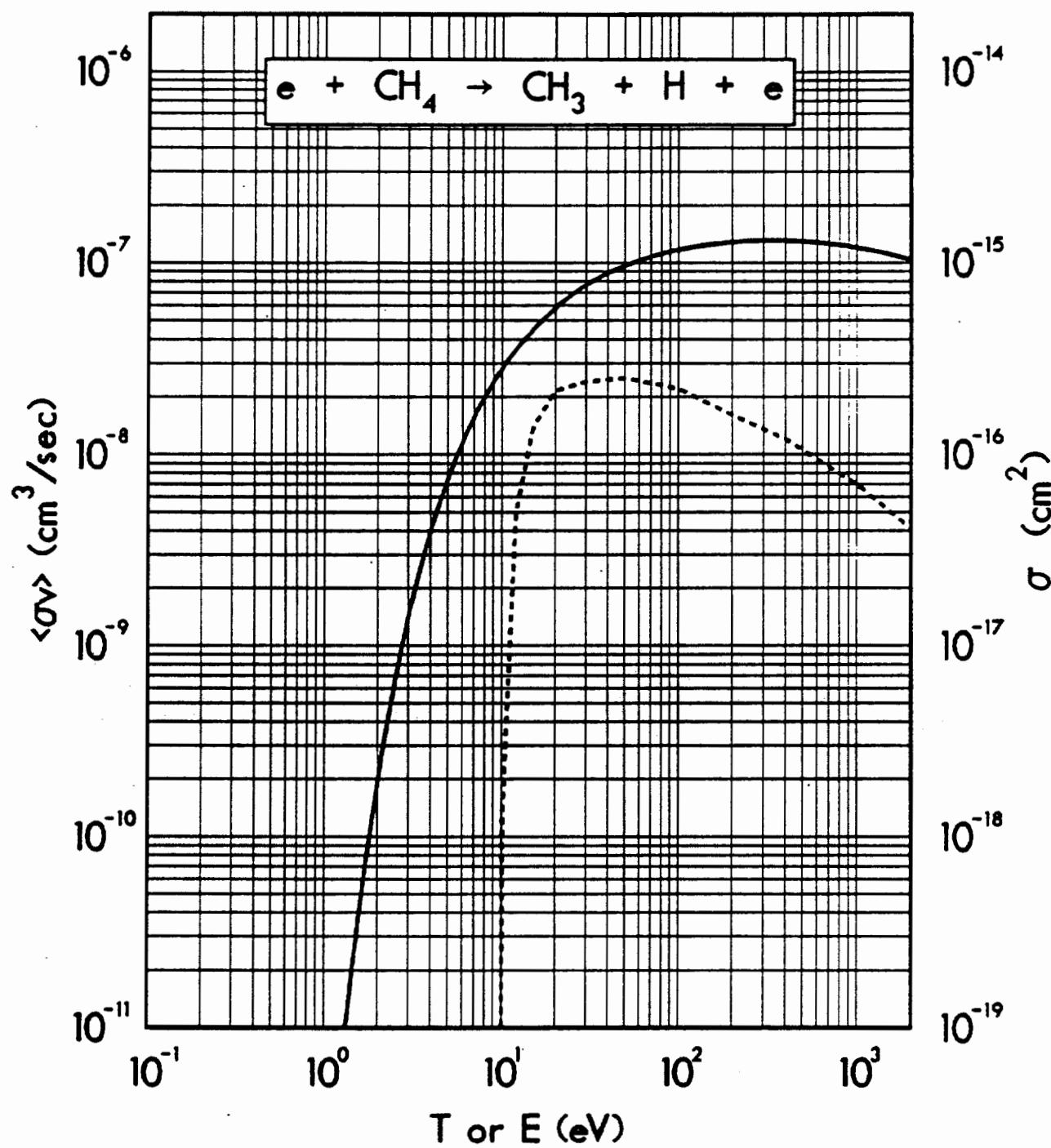
Energetics:

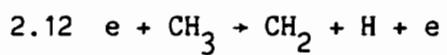
$$\Delta E_e^{(-)} \approx 10 \text{ eV}$$

$$\Delta E_H^{(+)} \approx 3 \text{ eV}$$

$$\Delta E_{\text{CH}_3}^{(+)} \approx 0.3 \text{ eV}$$

Comments: The dissociation cross section, σ_d , is derived by subtracting the measured dissociative ionization cross section from the total dissociation cross section measured by Winters (1975). Above 50 eV, the dissociation cross section is about half the total. Above 500 eV, a semiempirical extrapolation has been made using Winters' (1975) results.





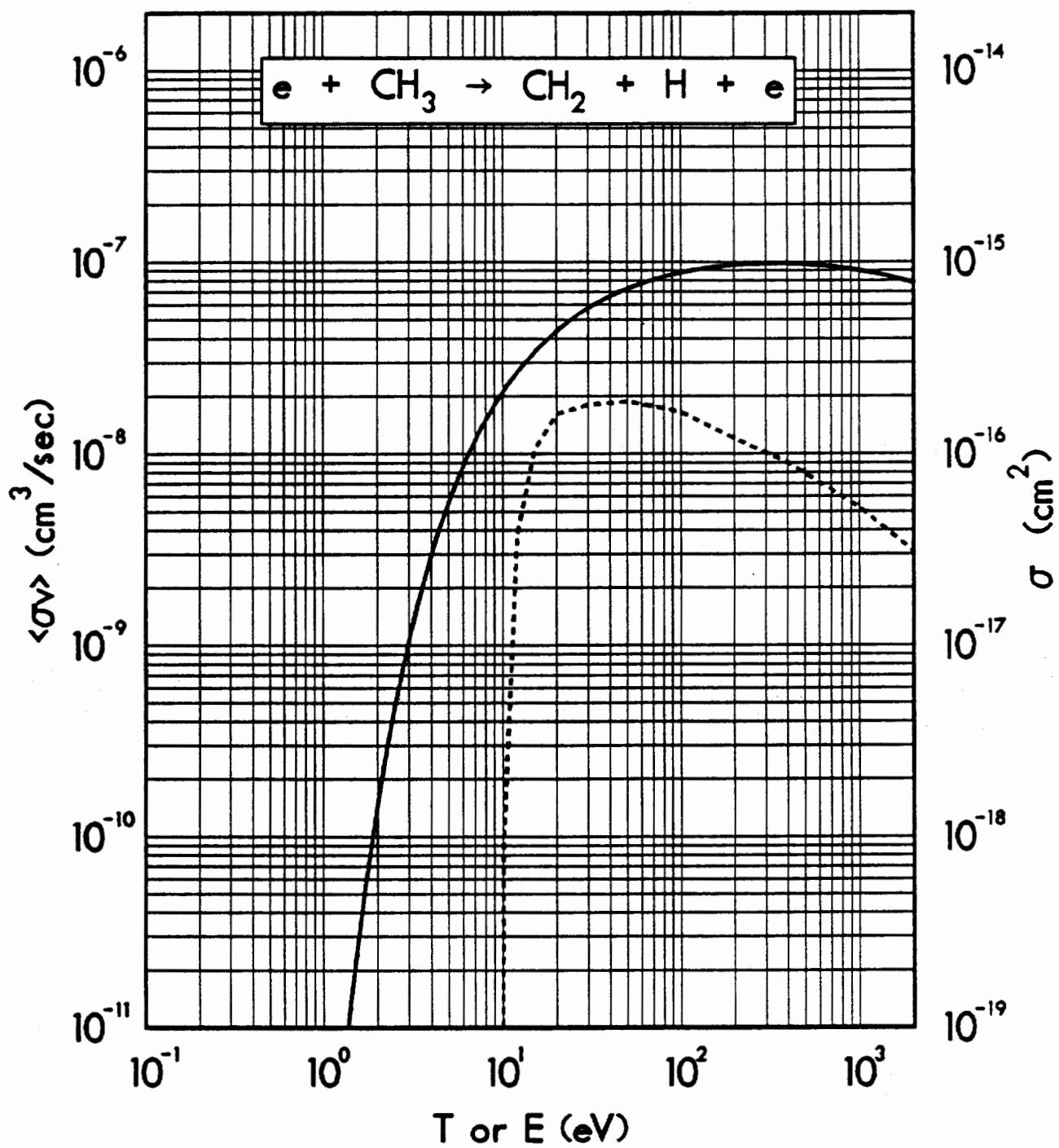
$$E_{\min} = 10 \text{ eV}$$

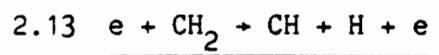
Cross Section:

$$\sigma_d = \frac{3}{4} \sigma_d (\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}) \text{ (reaction 2.11)}$$

Energetics: See reaction 2.11.

Comments: The dissociation of CH_3 is assumed to be $3/4$ that of CH_4 to take into account that there are proportionally fewer target hydrogen particles. This assumption is guided by the observation of a smaller cross section for dissociative ionization of CD_2 compared to CD_3 (Baiocchi et al. 1984). The energetics are taken to be the same as those of reaction 2.11.





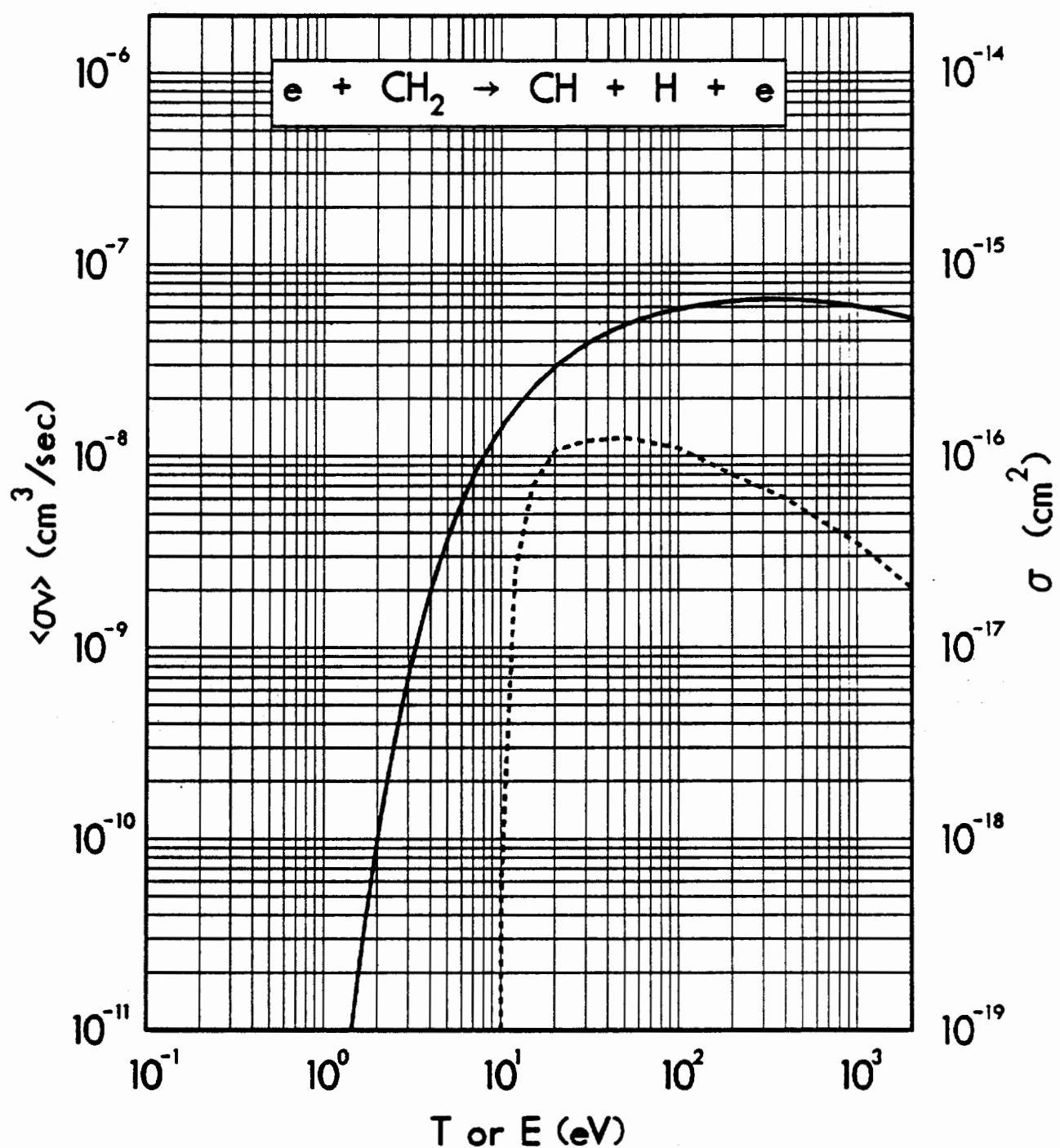
$$E_{\min} = 10 \text{ eV}$$

Cross Section:

$$\sigma_d = 1/2 \sigma_d (\text{CH}_4 + \text{CH}_3 + \text{H}) \text{ (reaction 2.11)}$$

Energetics: See reaction 2.11.

Comments: See comments for reaction 2.12.





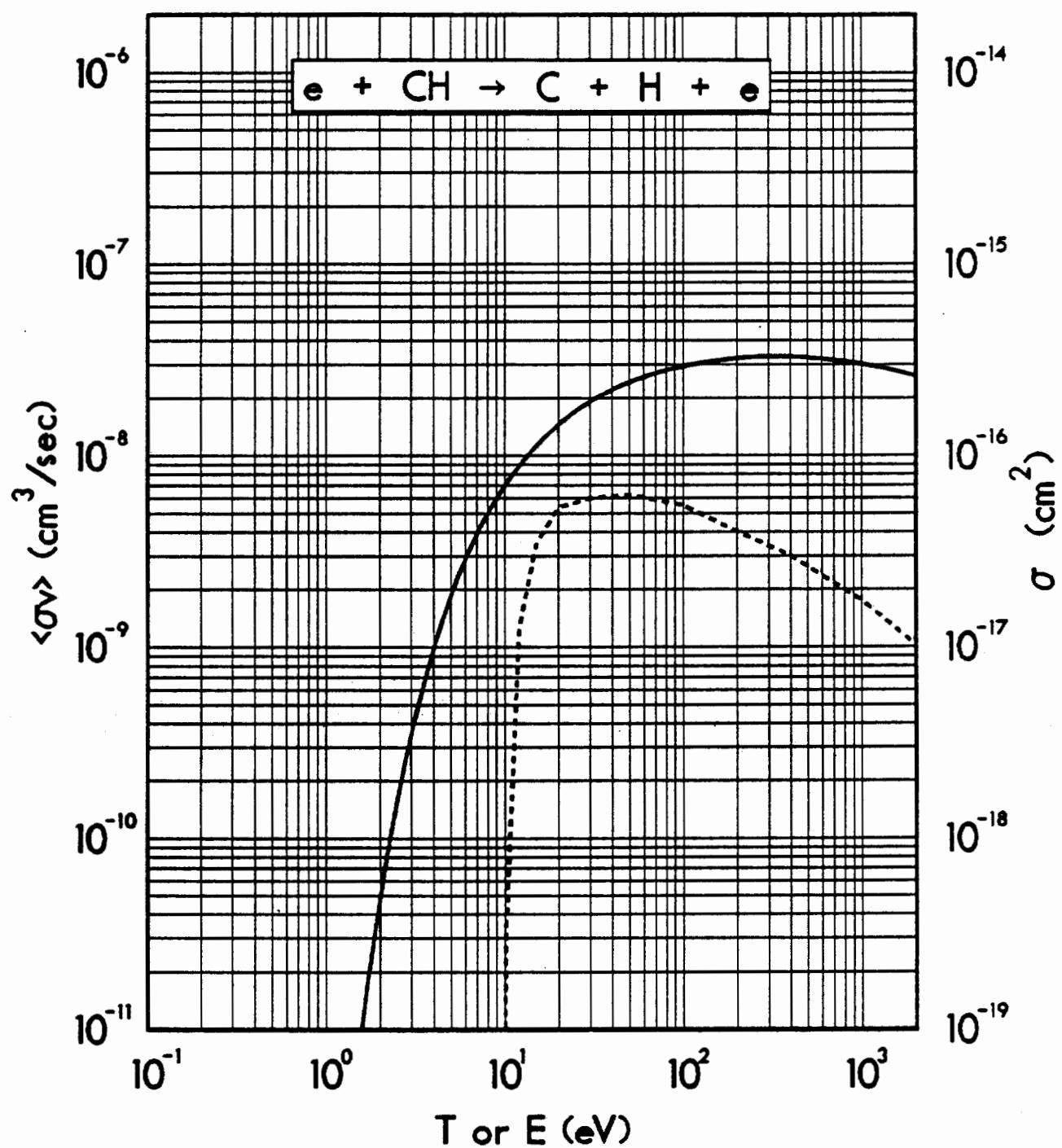
$E = 10 \text{ eV}$

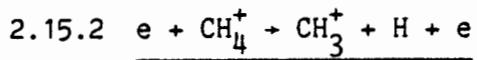
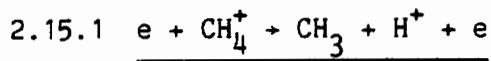
Cross Section:

$$\sigma_d = 1/4 \sigma_d (CH_4 \rightarrow CH_3 + H) \text{ (reaction 2.11)}$$

Energetics: See reaction 2.11.

Comments: See comments for reaction 2.12.





$$\langle E_{\min} \rangle = 10 \text{ eV}$$

Cross Sections:

$$2.15.1 \quad \sigma_d = \alpha \sigma_d(\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}) = \\ 1/4 \sigma_d(\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}) \quad (\text{reaction 2.11})$$

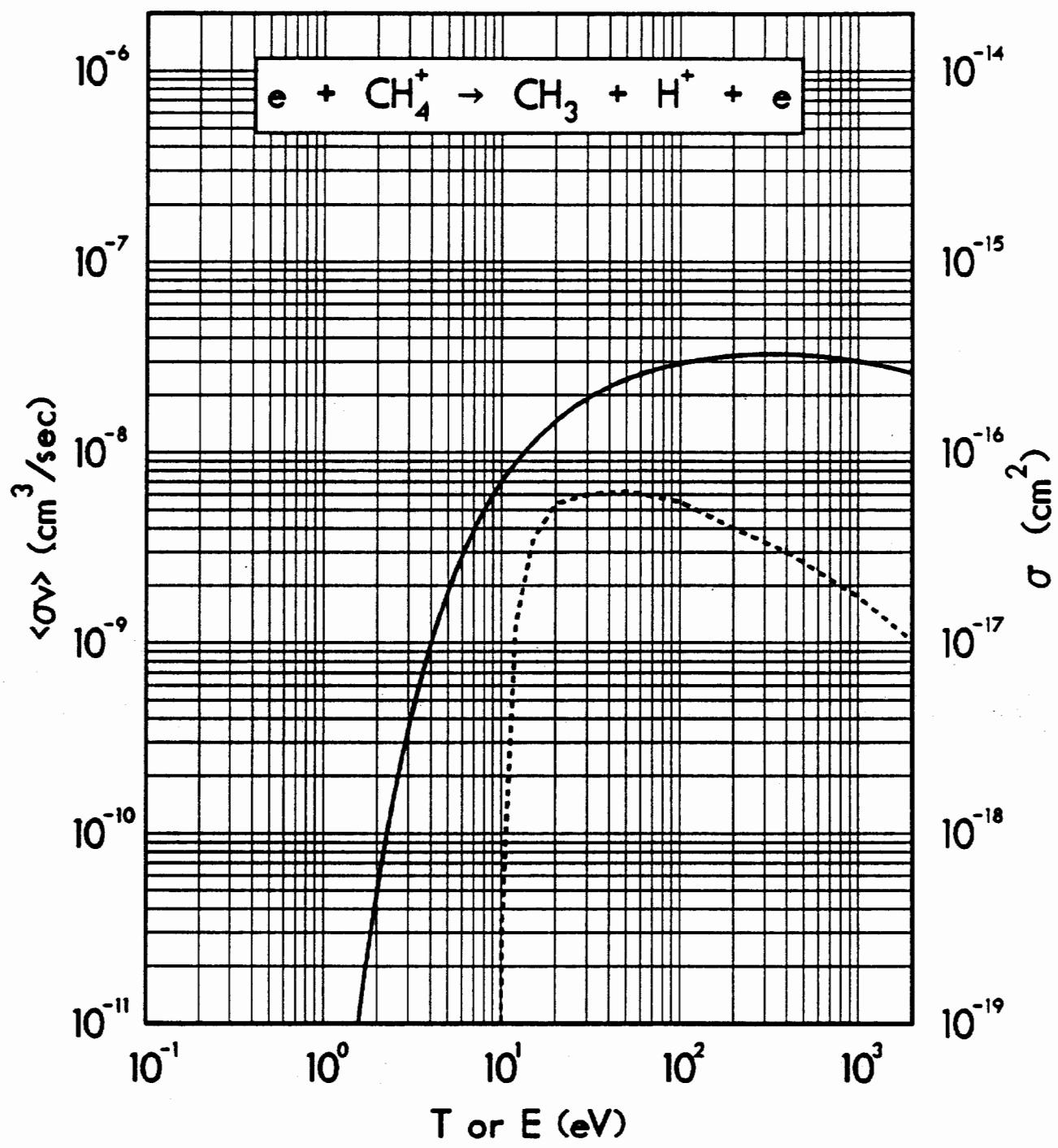
$$2.15.2 \quad \sigma_d = (1 - \alpha) \sigma_d(\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}) = \\ 3/4 \sigma_d(\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}) \quad (\text{reaction 2.11})$$

Energetics:

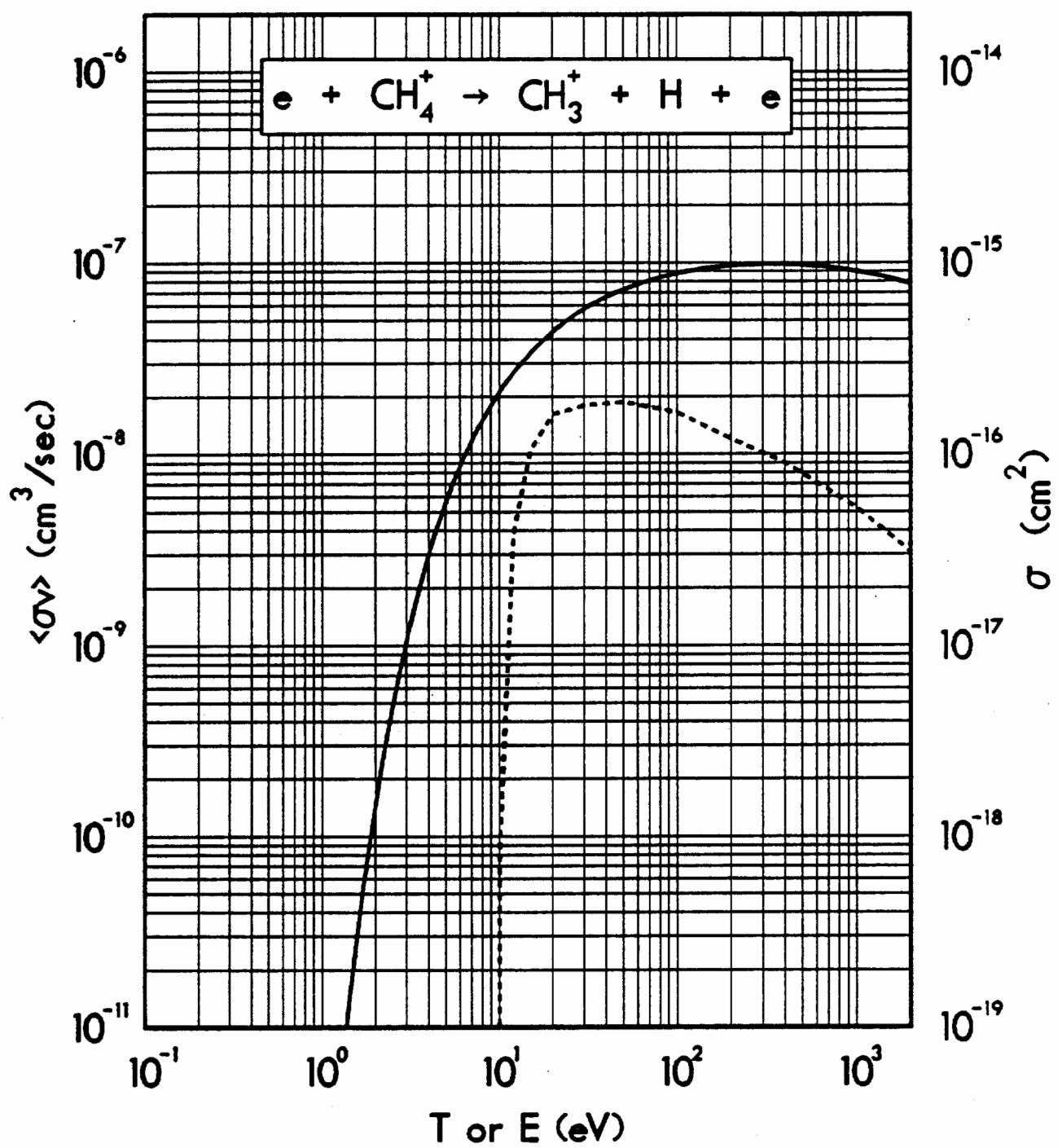
$$\Delta E_e^{(-)} = 14 \text{ eV}$$

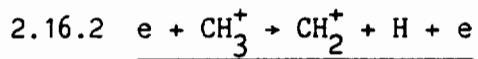
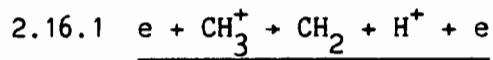
$$\Delta E_{(\text{H or H}^+)}^{(+)} \approx 3 \text{ eV} \quad \Delta E_{(\text{CH}_3 \text{ or } \text{CH}_3^+)}^{(+)} \approx 0.3 \text{ eV}$$

Comments: There are no direct measurements of these dissociation processes, but collision studies with energetic CH_4^+ in gases (Tunitskii, Kupriyanov, and Perov 1961) suggest that the total electron dissociation cross section is similar to that of methane. Furthermore, the distribution of final products appears related to the statistical distribution of internal states, with the primary channel the removal of one particle. Adopting such a statistical law, we assume that the probability of removing each hydrogen is equal, which leads to $\alpha = 1/4$ for the branching to reaction 2.15.1 and $(1 - \alpha) = 3/4$ to 2.15.2. The energetics are similar to those in reaction 2.5.



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$$\langle E_{\min} \rangle = 10 \text{ eV}$$

Cross Sections:

$$2.16.1 \quad \sigma_d = \alpha \sigma_d(\text{CH}_3 \rightarrow \text{CH}_2 + \text{H}) = \\ 1/3 \sigma_d(\text{CH}_3 \rightarrow \text{CH}_2 + \text{H}) \quad (\text{reaction 2.12})$$

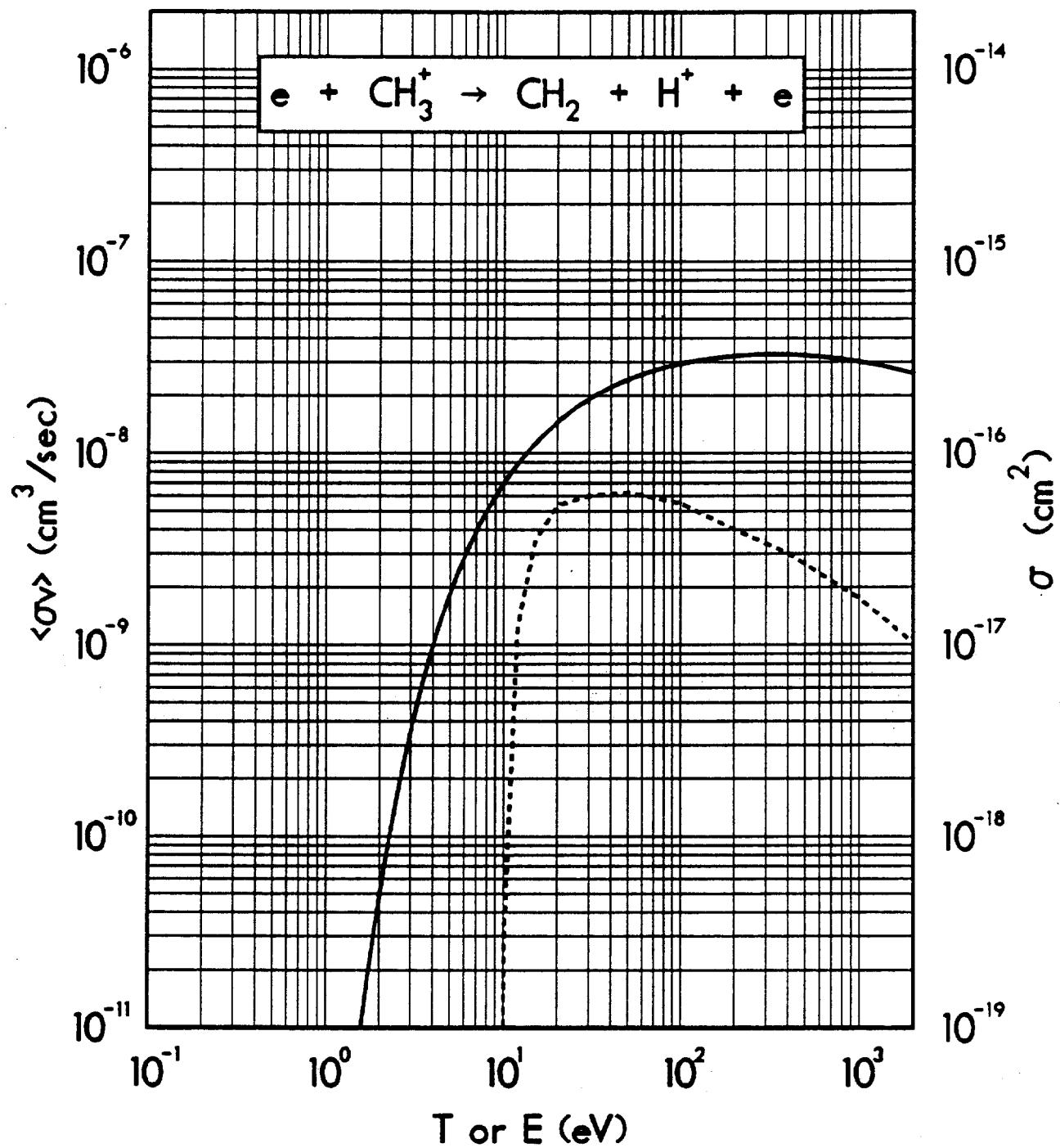
$$2.16.2 \quad \sigma_d = (1 - \alpha) \sigma_d(\text{CH}_3 \rightarrow \text{CH}_2 + \text{H}) = \\ 2/3 \sigma_d(\text{CH}_3 \rightarrow \text{CH}_2 + \text{H}) \quad (\text{reaction 2.12})$$

Energetics:

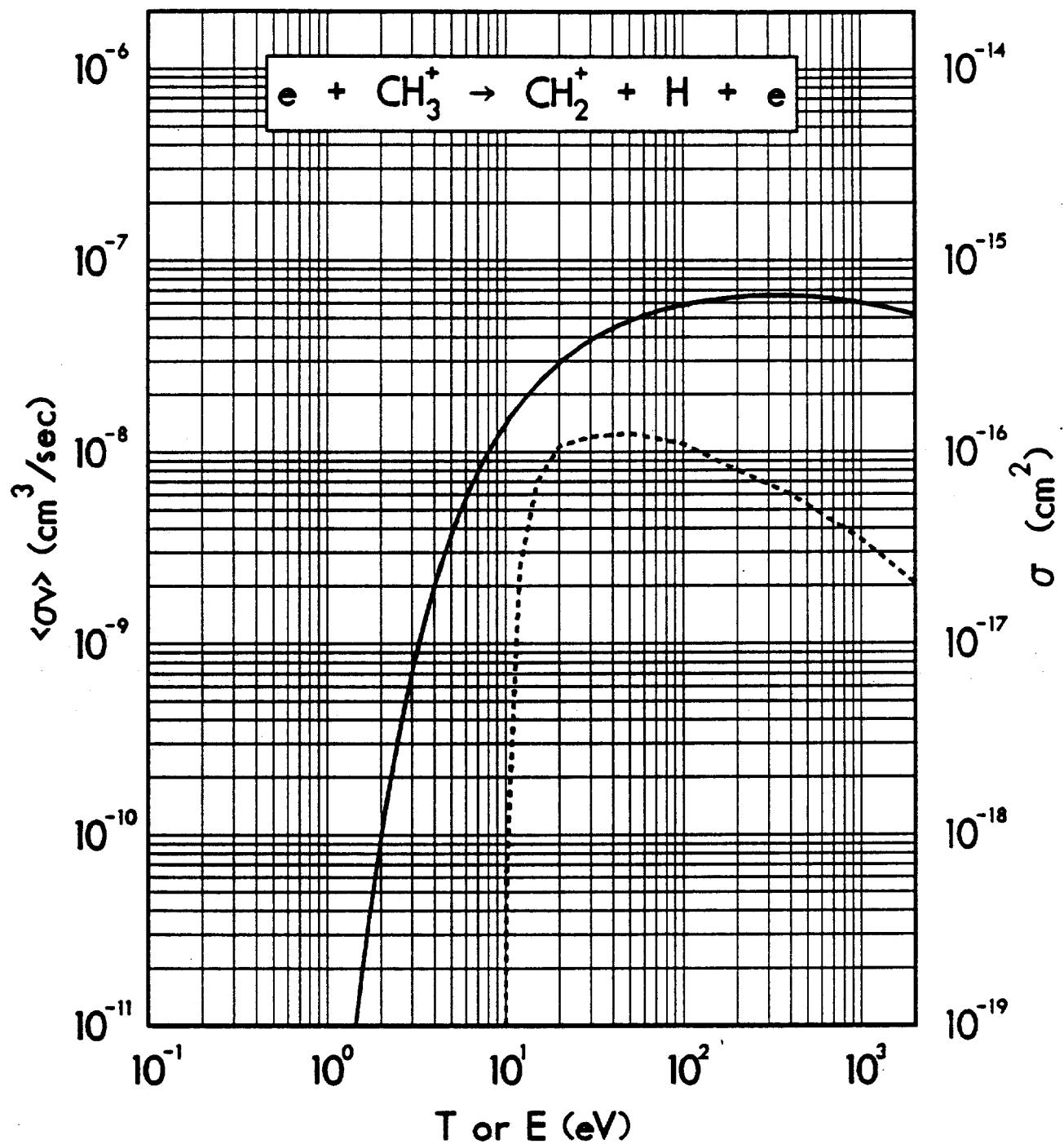
$$\Delta E_e^{(-)} = 14 \text{ eV}$$

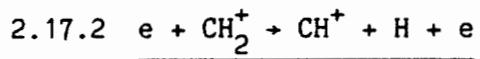
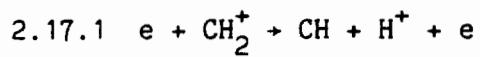
$$\Delta E_{(\text{H or H}^+)}^{(+)} \approx 3 \text{ eV} \quad \Delta E_{(\text{CH}_2 \text{ or } \text{CH}_3^+)}^{(+)} \approx 0.3 \text{ eV}$$

Comment: See the comments for reactions 2.15.1 and 2.15.2 for a discussion of the choice of branching parameter $\alpha = 1/3$ for reaction 2.16.1.



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$$\langle E_{\min} \rangle = 10 \text{ eV}$$

Cross Sections:

$$2.17.1 \quad \sigma_d = \alpha \sigma_d(\text{CH}_2 \rightarrow \text{CH} + \text{H}) = \\ 1/2 \sigma_d(\text{CH}_2 \rightarrow \text{CH} + \text{H}) \quad (\text{reaction 2.13})$$

$$2.17.2 \quad \sigma_d = (1 - \alpha) \sigma_d(\text{CH}_2 \rightarrow \text{CH} + \text{H}) = \\ 1/2 \sigma_d(\text{CH}_2 \rightarrow \text{CH} + \text{H}) \quad (\text{reaction 2.13})$$

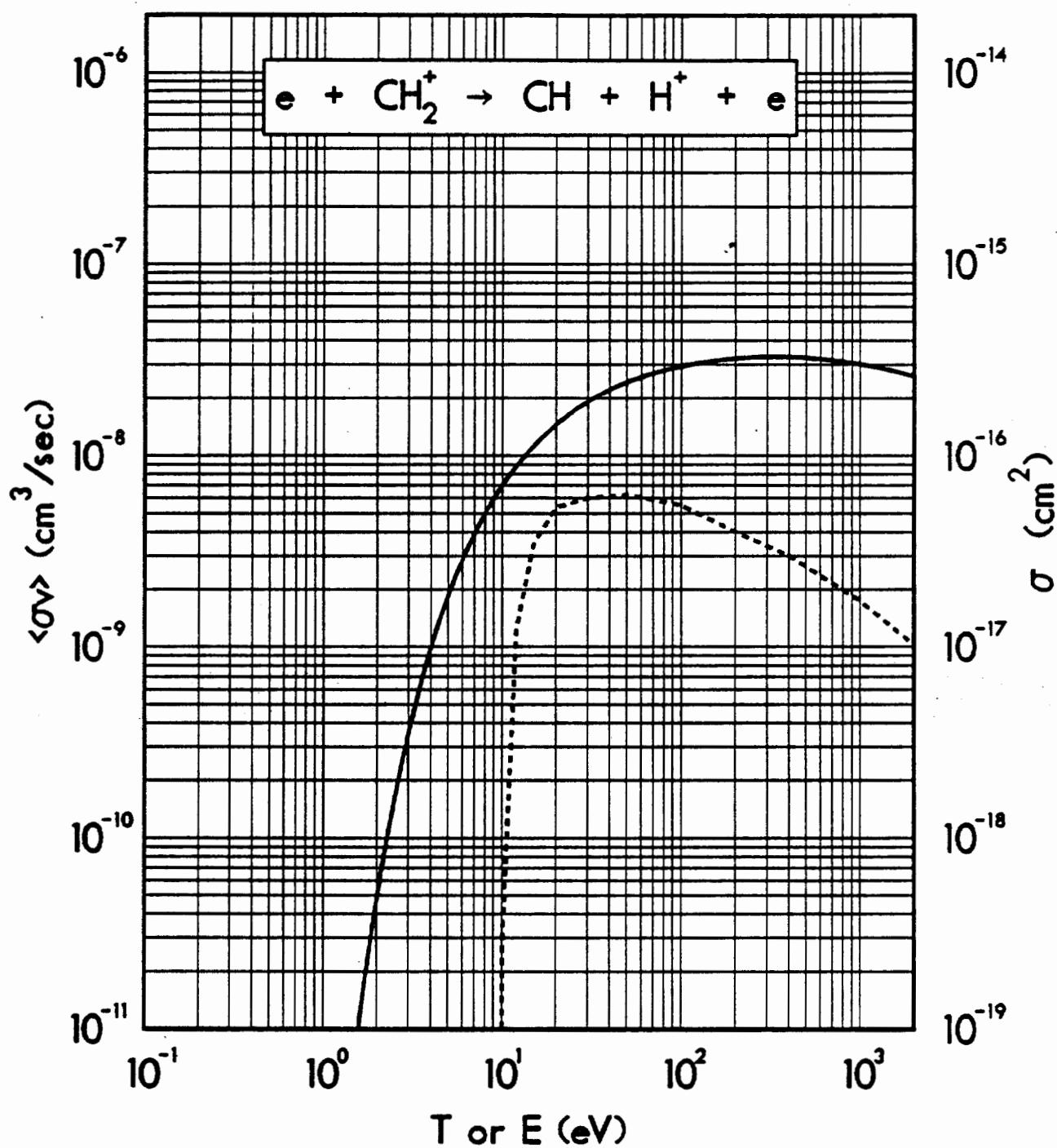
Energetics:

$$\Delta E_e^{(-)} = 14 \text{ eV}$$

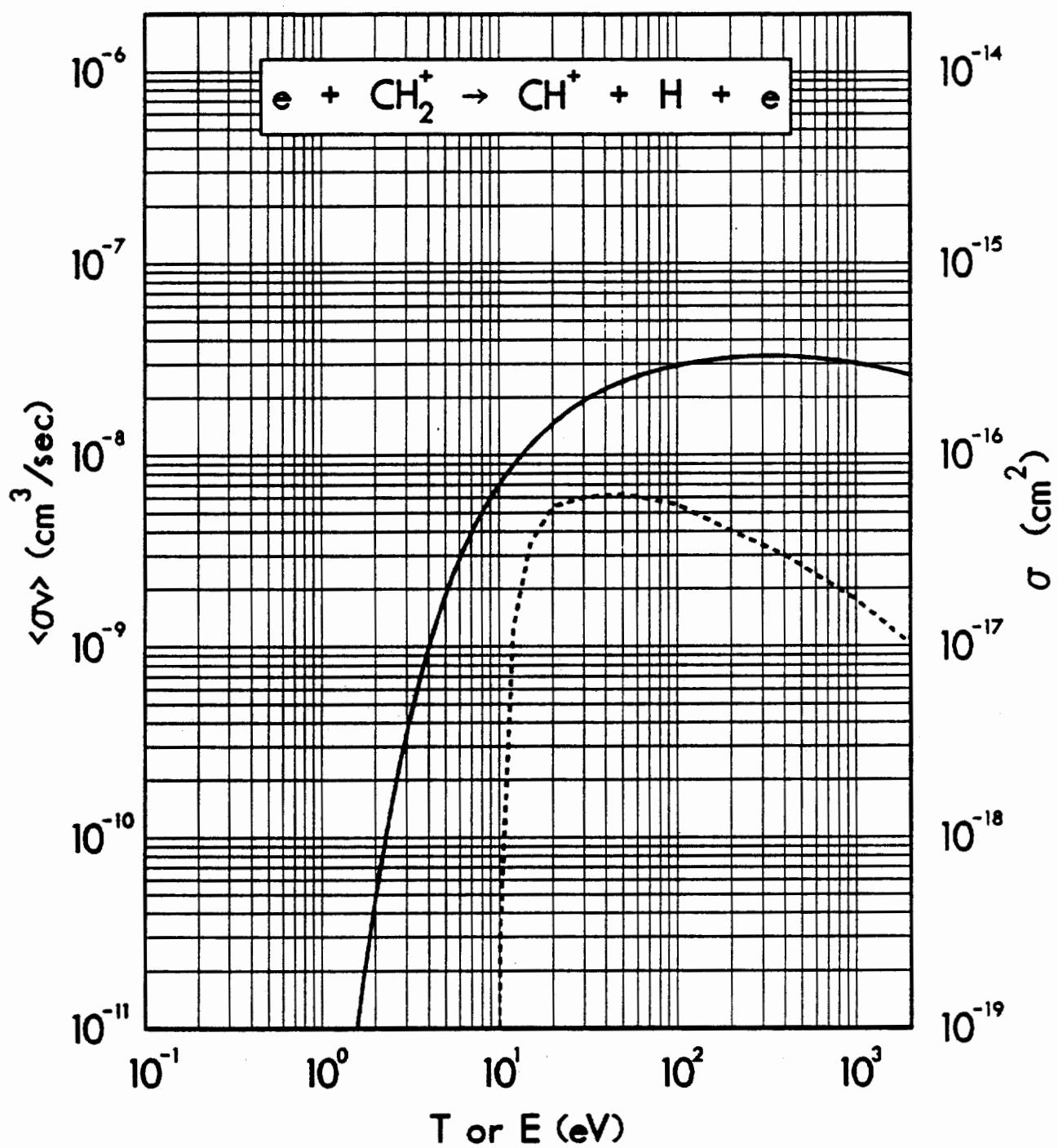
$$\Delta E_{(H \text{ or } H^+)}^{(+)} \approx 3 \text{ eV}$$

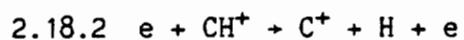
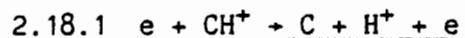
$$\Delta E_{(\text{CH or CH}^+)}^{(+)} \approx 0.3 \text{ eV}$$

Comments: See comments for reactions 2.15.1 and 2.15.2 for a discussion of the choice of branching parameter $\alpha = 1/2$ for reaction 2.17.1.



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$$\langle E_{\min} \rangle_{FC} = 10 \text{ eV}$$

Cross Sections:

$$2.18.1 \quad \sigma_d = \alpha \sigma_d(CH \rightarrow C + H) = \\ 1/2 \sigma_d(CH \rightarrow C + H) \quad (\text{reaction 2.14})$$

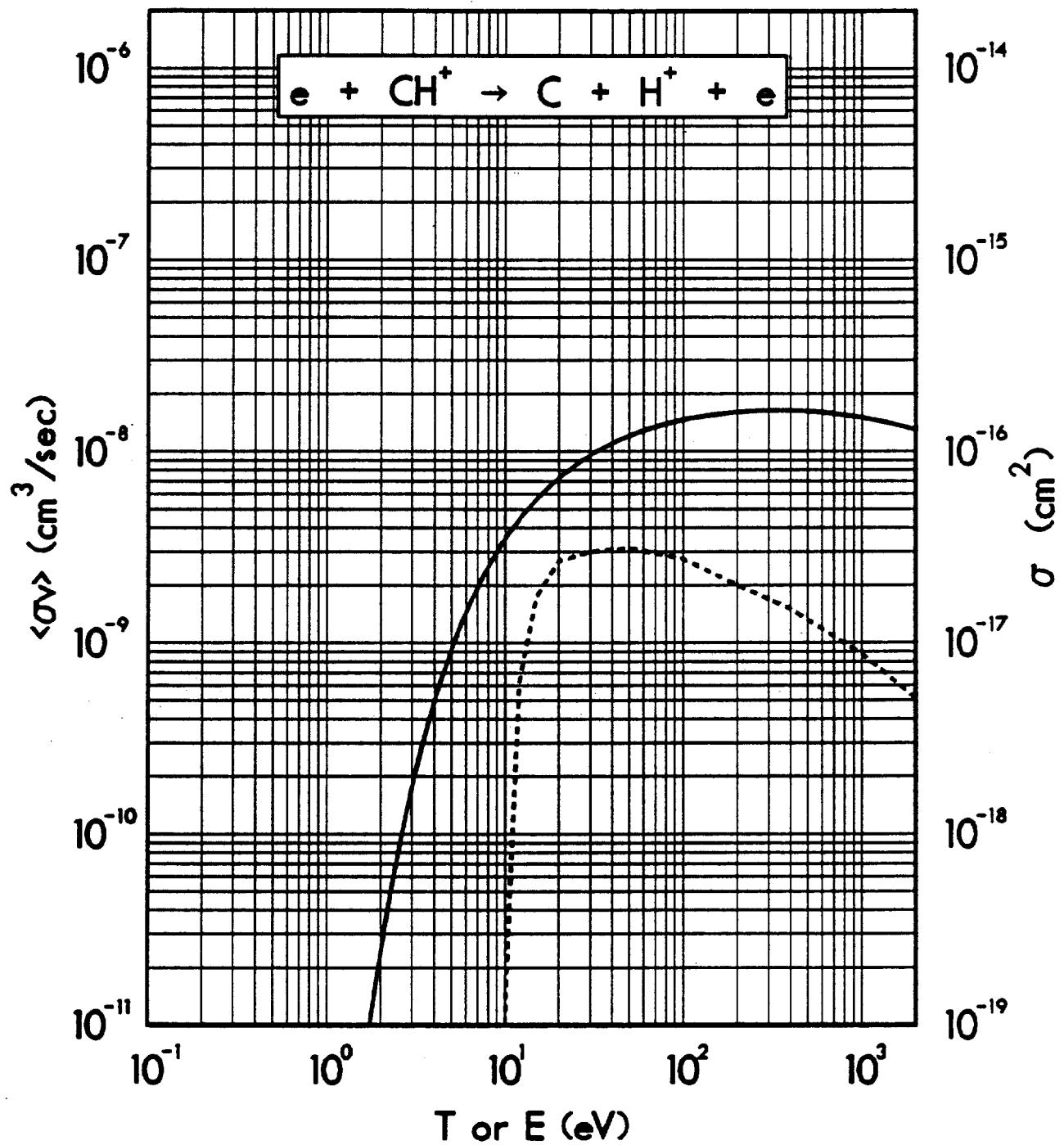
$$2.18.2 \quad \sigma_d = (1 - \alpha) \sigma_d(CH \rightarrow C + H) = \\ 1/2 \sigma_d(CH \rightarrow C + H) \quad (\text{reaction 2.14})$$

Energetics:

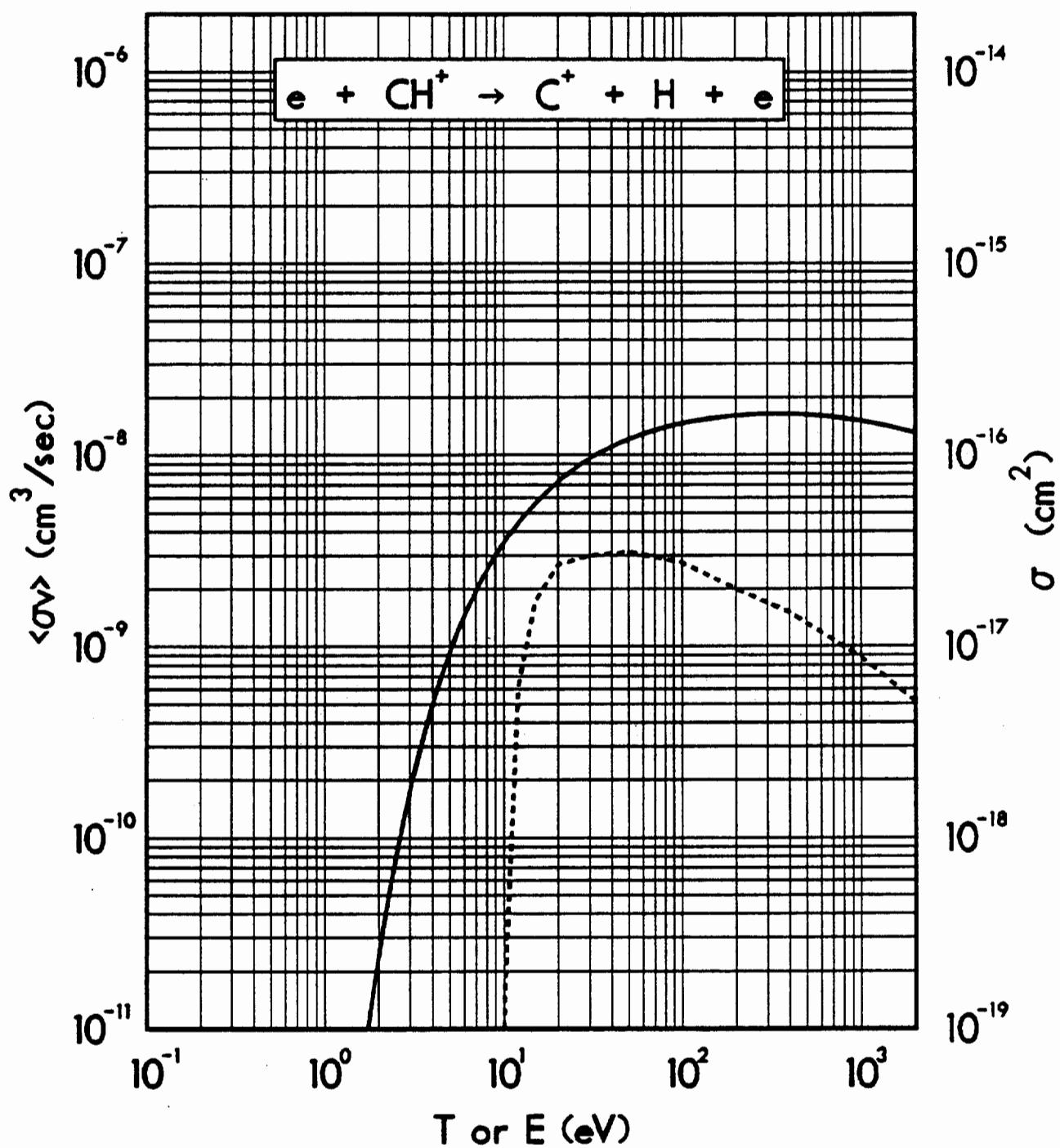
$$\Delta E_e^{(-)} = 14 \text{ eV}$$

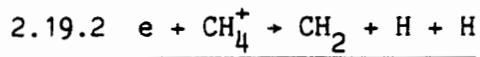
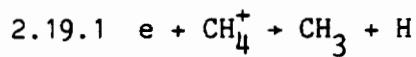
$$\Delta E_{(H \text{ or } H^+)}^{(+)} \approx 3 \text{ eV} \quad \Delta E_{(C \text{ or } C^+)}^{(+)} \approx 0.3 \text{ eV}$$

Comments: See comments for reactions 2.15.1 and 2.15.2 for a discussion of the choice of branching parameter α for reaction 2.18.1.



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$$E_{th} = 0 \text{ eV}$$

Cross Sections:

$$E < 0.1 \text{ eV}$$

$$\sigma_{dr}^{tot} = \sigma_{exp} = 2 \times 10^{-15} E^{-1} \text{ cm}^2$$

$$0.1 < E < 1 \text{ eV}$$

$$\sigma_{dr}^{tot} = \sigma_{exp} = 5 \times 10^{-16} E^{-1.6} \text{ cm}^2$$

$$E > 1 \text{ eV}$$

$$\sigma_{dr}^{tot} = \sigma_{se} \propto E^{-1.6}$$

References: Mul et al. (1981)

Energetics:

$$\Delta E_e^{(-)} = E$$

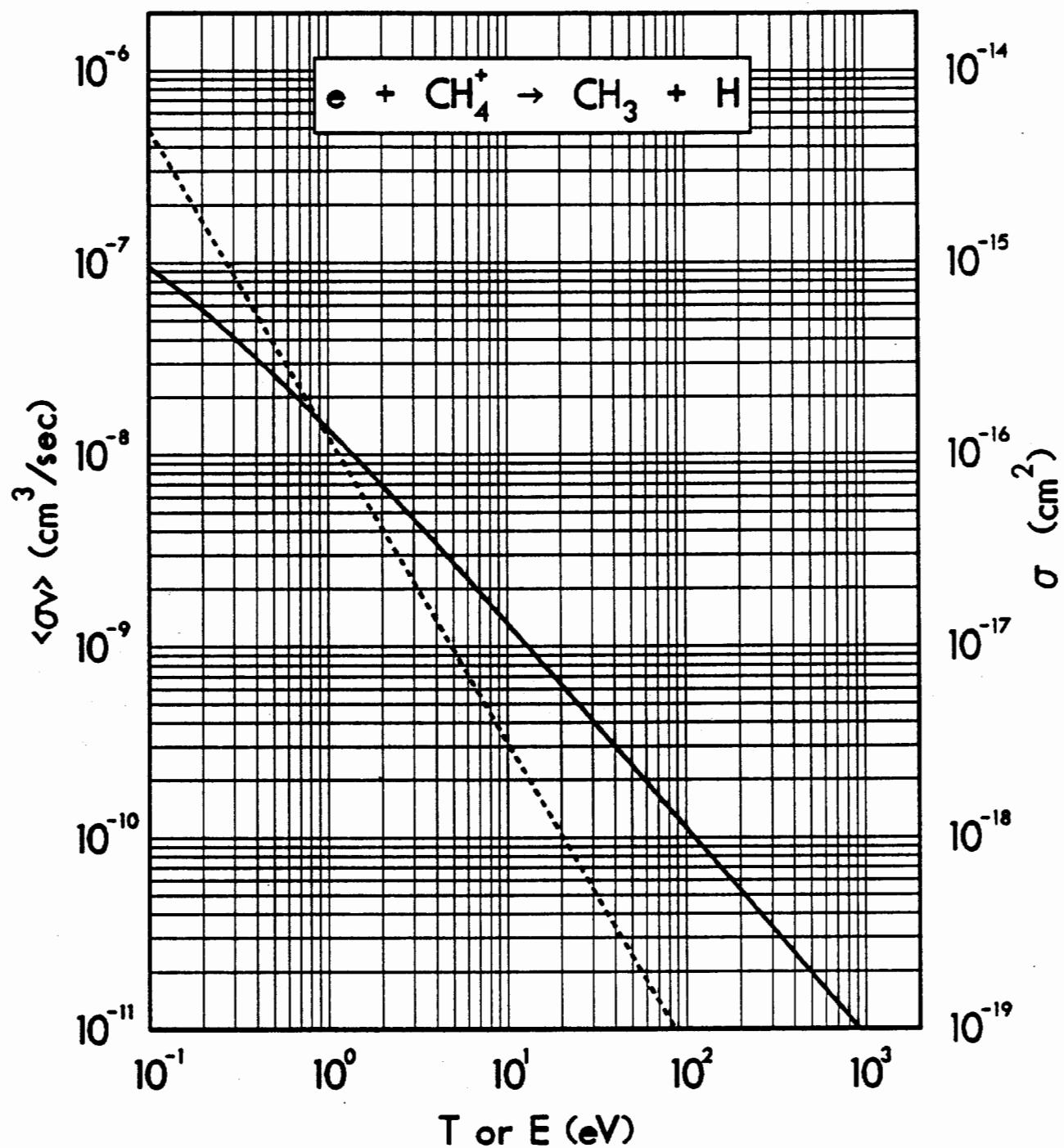
$$\langle \Delta E_{\text{CH}_m}^{(+)} \rangle \approx 0.1 E$$

2.19.1 $\langle \Delta E_{\text{H}}^{(+)} \rangle \approx 0.9 E$

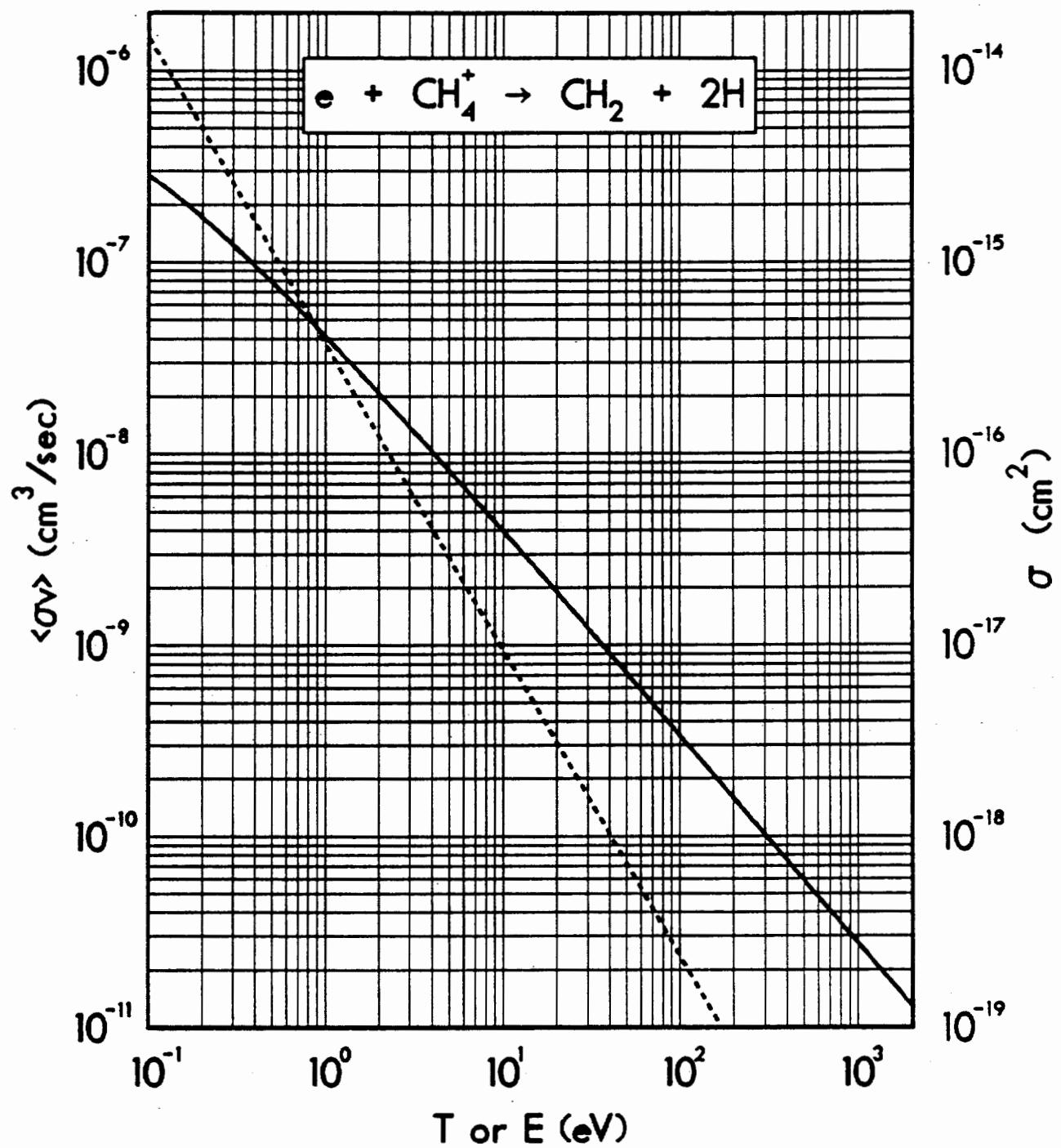
2.19.2 $\langle \Delta E_{\text{H}}^{(+)} \rangle \approx 0.45 E$

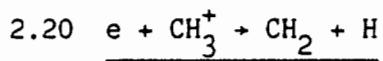
Comments:

- (1) The energy dependence beyond 1 eV is extrapolated from the low energy measurements. Above 10 eV, the cross sections are likely to be overestimated by σ_{se} as other competing channels become more important.
- (2) According to Bates (1986), the recombination to CH_2 is probably the dominant channel, and we have selected a weight of 3/4 for this branch with a weight of 1/4 for 2.19.1.



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$$E_{th} = 0 \text{ eV}$$

Cross Sections:

$$E < 0.1$$

$$\sigma_{dr}^{tot} = \sigma_{exp} = 2 \times 10^{-15} E^{-1} \text{ cm}^2$$

$$0.1 < E < 1.0 \text{ eV}$$

$$\sigma_{dr}^{tot} = \sigma_{exp} = 7 \times 10^{-16} E^{-1.5} \text{ cm}^2$$

$$e > 1.0 \text{ eV}$$

$$\sigma_{dr}^{tot} = \sigma_{se} \propto E^{-1.5} \text{ cm}^2$$

References: Mul et al. (1981)

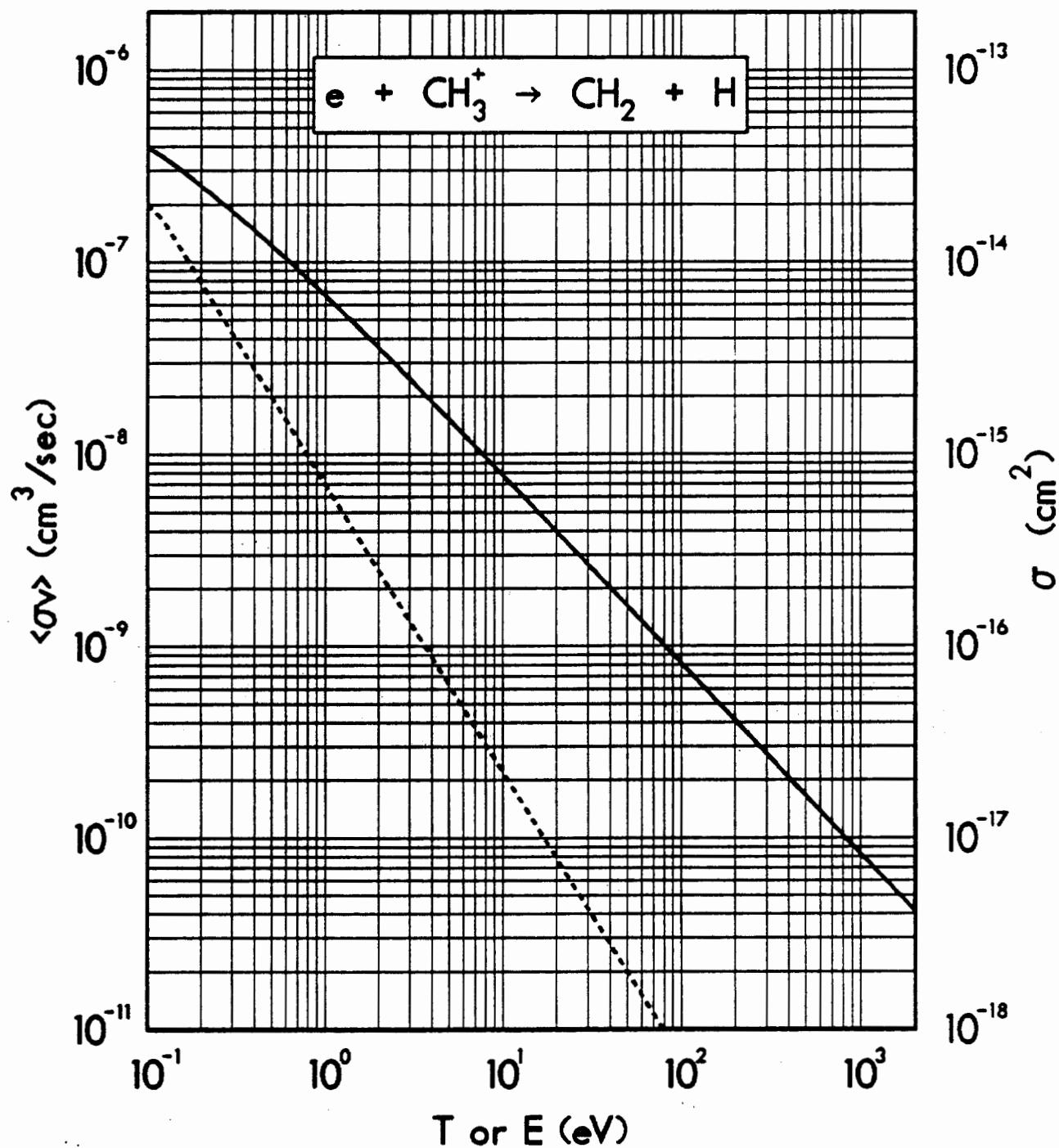
Energetics:

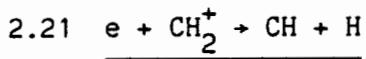
$$\Delta E_e^{(-)} = E$$

$$\Delta E_H^{(+)} \approx 0.9 E$$

$$\Delta E_{\text{CH}_2}^{(+)} \approx 0.1 E$$

Comments: The dominant recombination is to $\text{CH}_2 + H$ (Bates 1986), and we neglect any other channels.





$$E_{th} = 0$$

Cross Sections:

$$E < 1.0 \text{ eV}$$

$$\sigma_{dr}^{\text{tot}} = \sigma_{\text{exp}} = 1.7 \times 10^{-15} E^{-1} \text{ cm}^2$$

$$E > 1.0 \text{ eV}$$

$$\sigma_{dr}^{\text{tot}} = \sigma_{se} \propto E^{-2}$$

References: Mul et al. (1981)

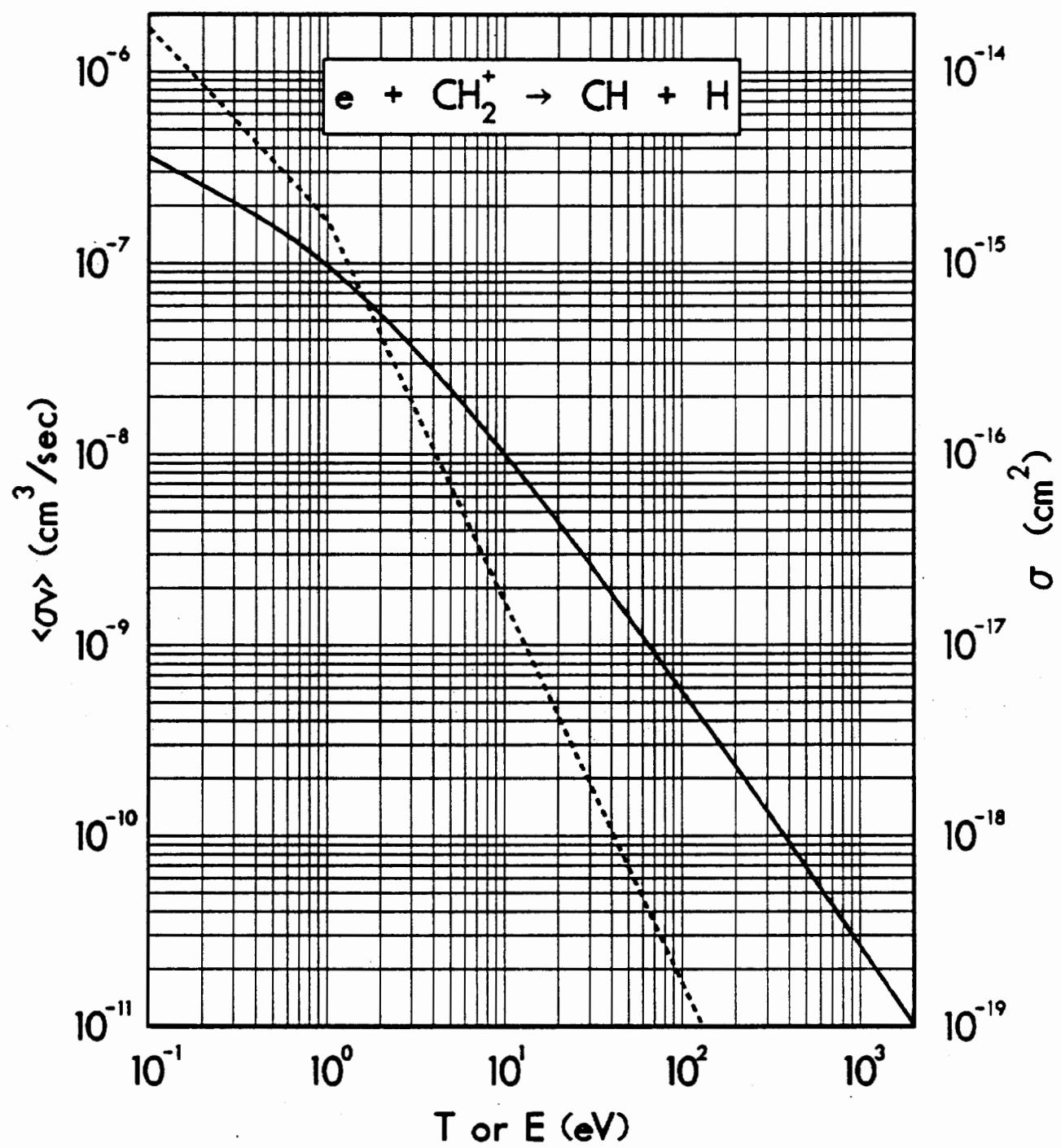
Energetics:

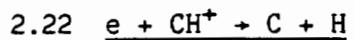
$$\Delta E_e^{(-)} = E$$

$$\Delta E_H^{(+)} \approx 0.9 E$$

$$\Delta E_{\text{CH}}^{(+)} \approx 0.1 E$$

Comments: The measured energy dependence up to 1 eV shows a nearly E^{-1} behavior. Above this energy, we have assumed an E^{-2} dependence as indicated by the break seen for several species (Mul and McGowan 1979; Mul et al. 1981; Mul et al. 1983) and, perhaps, attributable to vibrational excitation of the target ion (Mul et al. 1981). The dominant recombination is to $\text{CH} + \text{H}$ (Bates 1986), and we neglect other channels.





$$E_{th} = 0 \text{ eV}$$

Cross Sections:

$$E < 1 \text{ eV}$$

$$\sigma_{dr}^{tot} = \sigma_{exp} = 1.2 \times 10^{-15} E^{-1} \text{ cm}^2$$

$$E > 1 \text{ eV}$$

$$\sigma_{dr}^{tot} \propto E^{-2}$$

References: Mul et al. (1981)

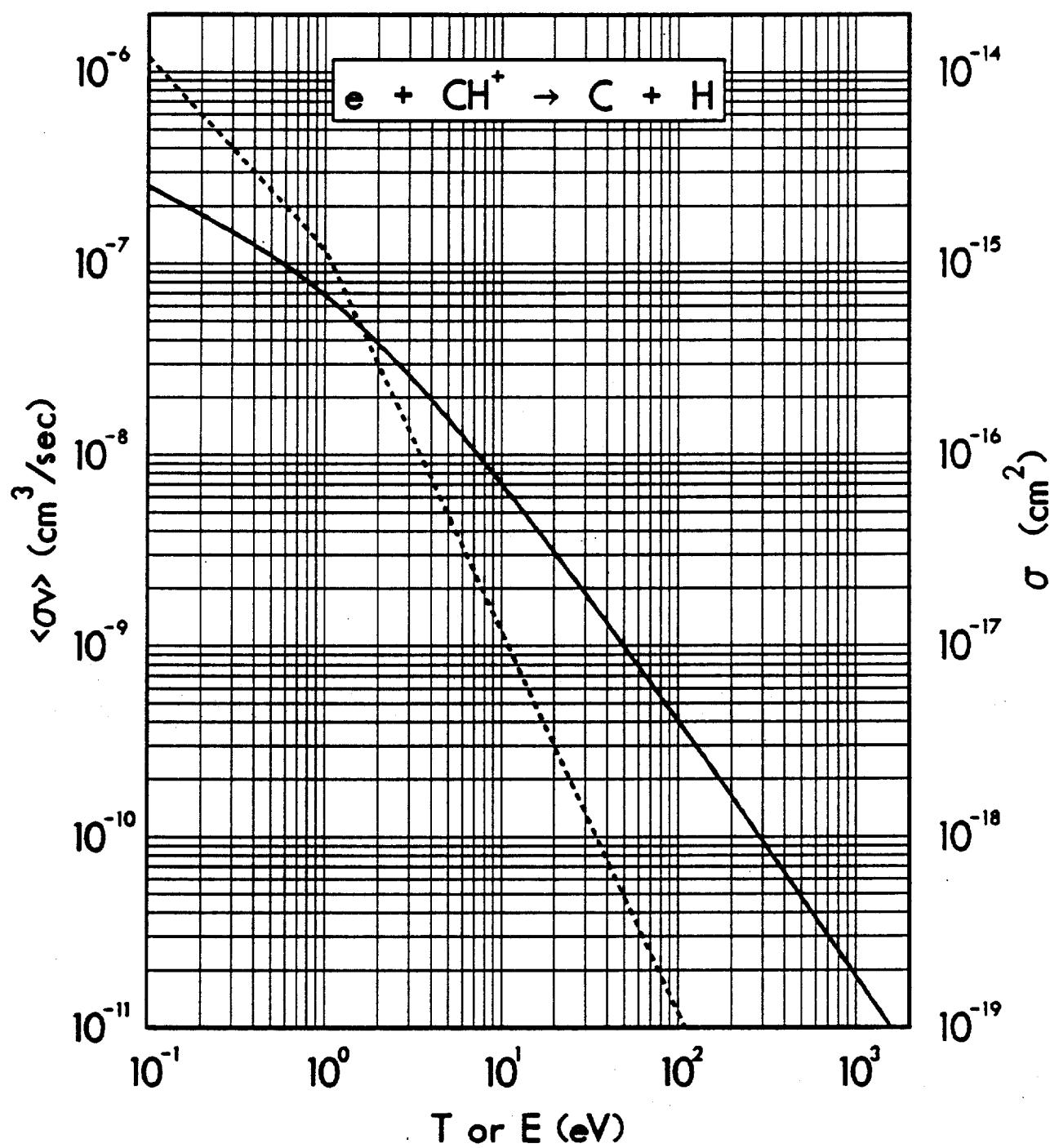
Energetics:

$$\Delta E_e^{(-)} = E$$

$$\Delta E_H^{(+)} \approx 0.9 E$$

$$\Delta E_C^{(+)} \approx 0.1 E$$

Comments: We have adopted an E^{-2} dependence for σ above 1 eV based on the observation that most polyatomic ions show such behavior although usually above about 0.2 eV. Above 10 eV, direct dissociation should compete with dissociative recombination.





$$E_{th} = 11.3 \text{ eV}$$

Cross Sections:

$$15 < E < 1500 \text{ eV}$$

$$\sigma_{ion} = \sigma_{exp}$$

$$E > 1500 \text{ eV}$$

$$\sigma_{ion} = \sigma_{se}$$

References: Barnett et al. (1977)

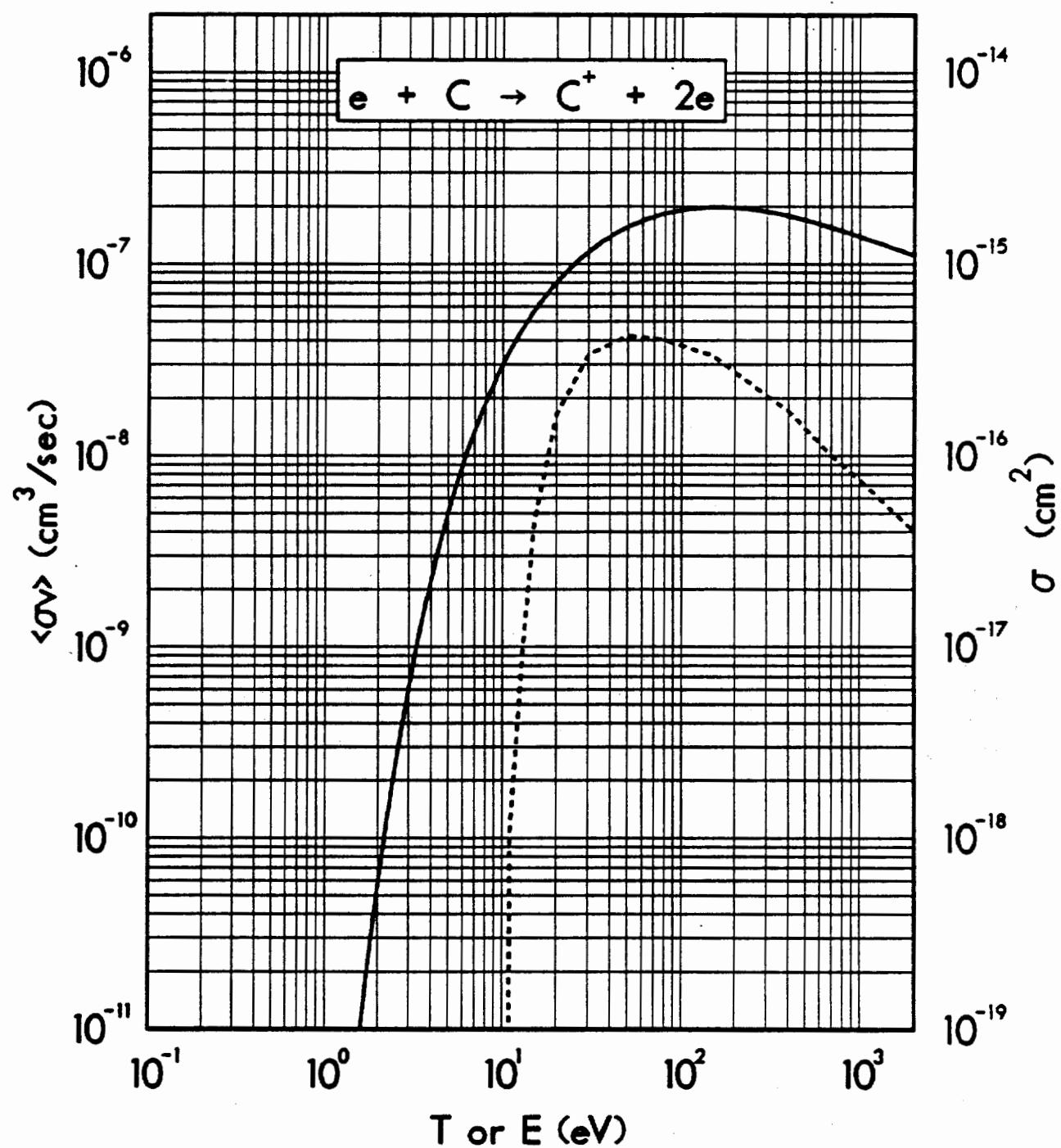
Energetics:

$$\Delta E_e^{(-)} = E_{th} + \langle E_{e'} \rangle$$

$$\langle E_{e'} \rangle = 1/2 (E - E_{th}), \quad E < 3/2 E_{th}$$

$$= 1/4 E_{th}, \quad E > 3/2 E_{th}$$

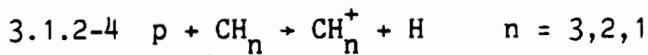
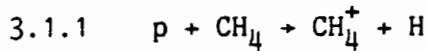
Comments: For a discussion of the energetics, see Janev et al. (1987) in the case of ionization of H(1s). σ_{se} is a semiempirical extrapolation based on Born dependence at higher energies (cf. Lotz 1967).



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3. PROTON IMPACT COLLISION REACTIONS

3. PROTON IMPACT COLLISION REACTIONS



$$E_{th} = 0 \text{ eV}$$

Cross Sections:

$$E > 100 \text{ eV} \quad \sigma_{cx} = \sigma_{exp}$$

$$0.03 < E < 100 \text{ eV} \quad \sigma_{cx} = \sigma_{ext}$$

$$E < 0.03 \text{ eV} \quad \sigma_{cx} = \sigma_{exp}$$

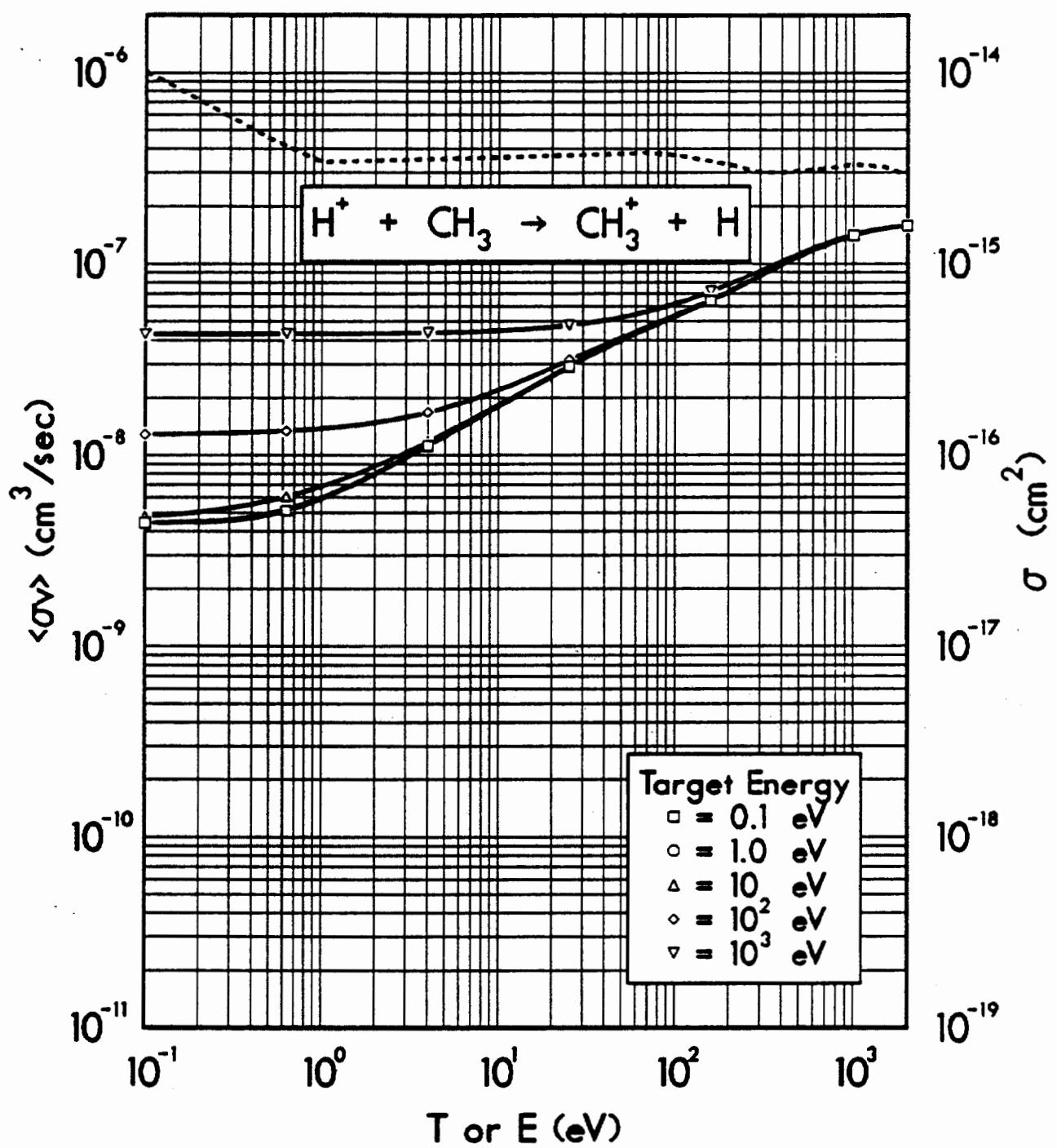
References: Nakai et al. (1983); Prasad and Huntress (1980)

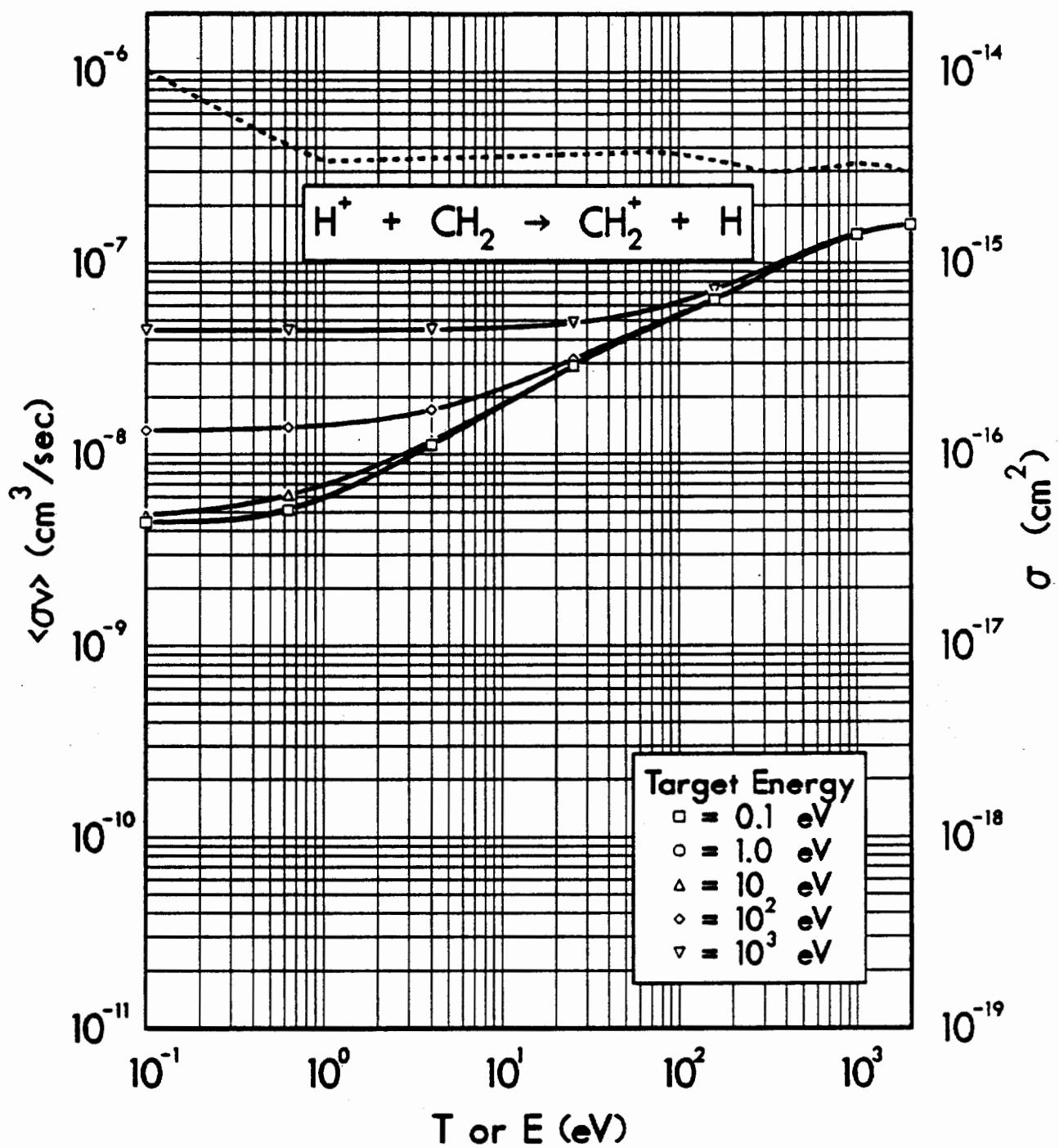
Energetics:

$$\Delta E_p^{(-)} = 0 \text{ eV} \quad \Delta E_{CH_n^+}^{(+)} = 0 \text{ eV}$$

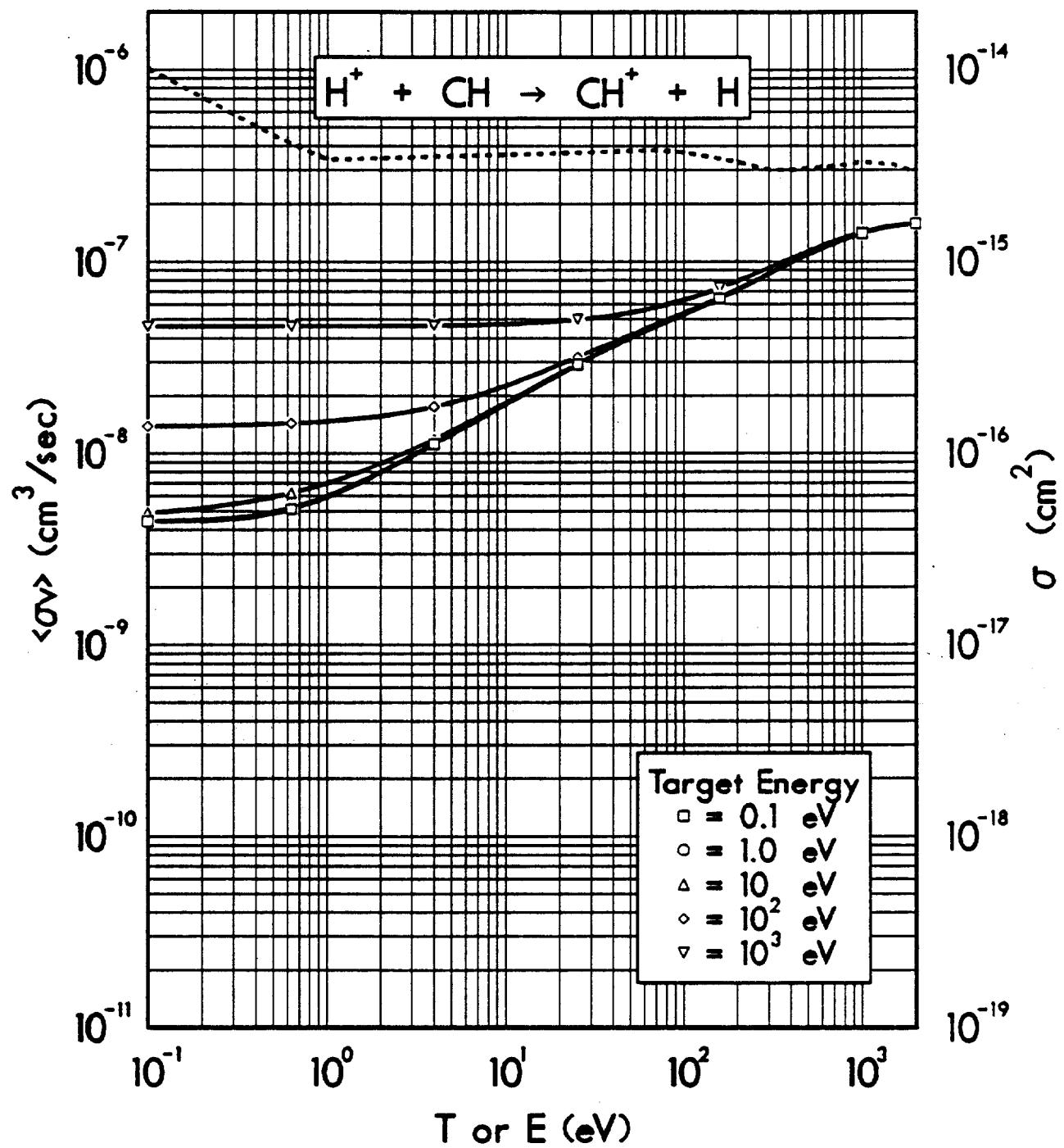
Comments: The low energy room temperature data have been extrapolated up to 1 eV at which point they match a nearly constant extrapolation of the high energy results. We have combined the two dominant channels at low temperature, $+ CH_4^+ + H$ and $CH_3^+ + H_2$, into one channel for purposes of determining the total cross section.

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3.2 $p + C \rightarrow C^+ + H$

$$E_{th} = 0.0 \text{ eV}$$

Cross Sections:

$$E > 50 \text{ eV}$$

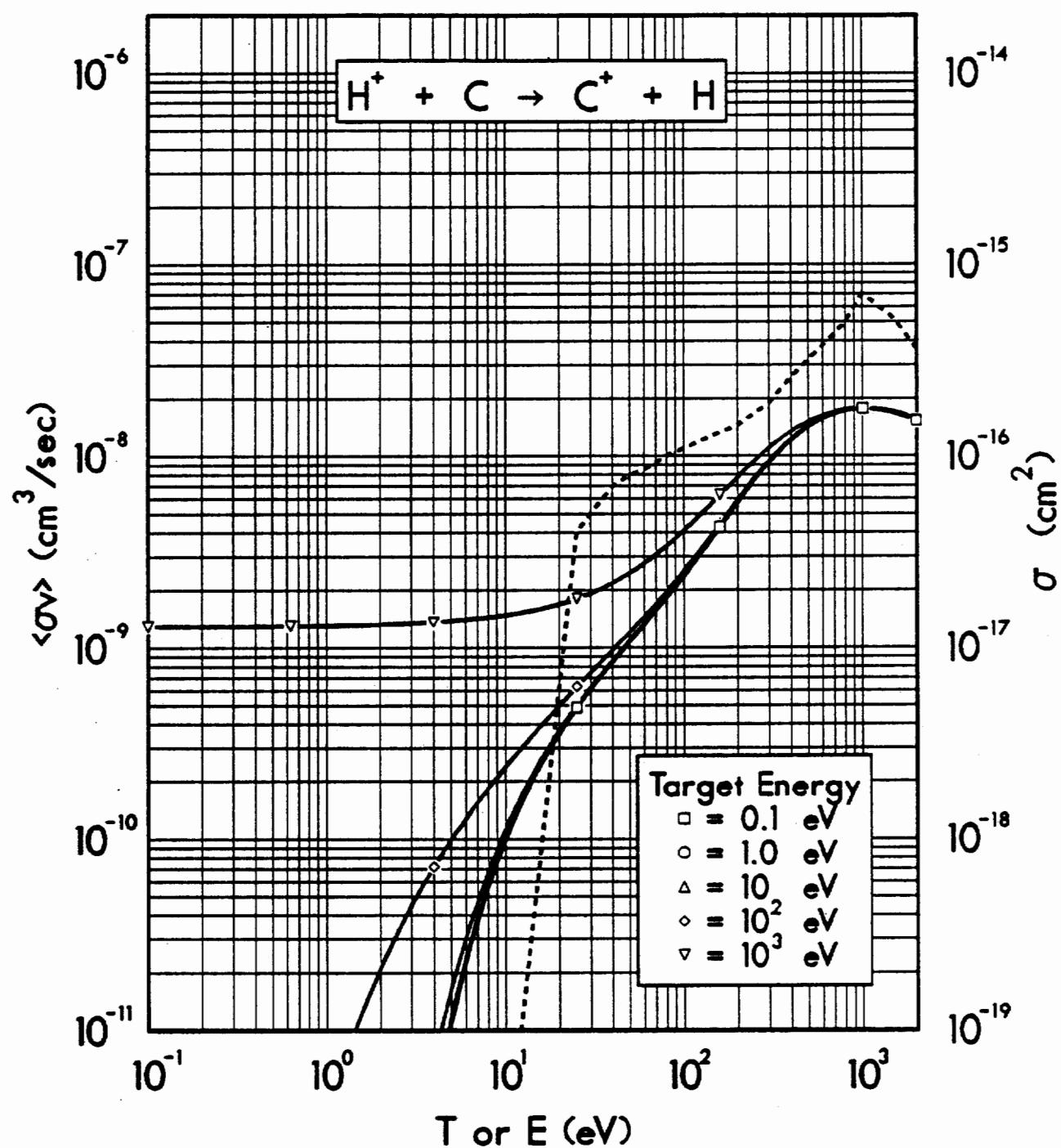
$$\sigma_{cx} = \sigma_{exp}$$

$$E \approx 1 \text{ eV}$$

$$\sigma_{cx} = \sigma_{th}$$

References: Nutt et al. (1979), Greenland (1984), Butler and Dalgarno (1980)

Comments: It was necessary to assume a very sharp cutoff at about 20 eV to extrapolate the experimental cross section down to the 1 eV theoretical value. The cross sections at these intermediate energies (1-50 eV) should be considered very uncertain at present.



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4. ANALYTIC FITS

In this chapter, we present analytic fits for σ and $\langle\sigma v\rangle$ as functions of energy and temperature. The coefficients contain 13 digits although, in most cases, fewer digits are sufficient.

It is strongly suggested that the user plot the fitted functions over the complete range of interest and compare them with the graphs contained in this report before using the fits, as the behavior of particular fits may make them unsuitable over part of the range from 0.1 to 2000 eV. In particular, the polynomial fits should not be used below the energy threshold, and the fitted reaction rate coefficients should not be used below T_{min} .

4.1 Fits for σ

We fit all cross sections with a 9-term (8th-order) polynomial,

$$\ln \sigma = \sum_{n=0}^8 a_n (\ln E)^n .$$

The coefficients were determined by a least-squares match of the fit to the data with weighting designed to de-emphasize the points in the steep part of the curve. The tables list the coefficients a_n for all the reactions. In many cases, it is difficult to obtain the fits near threshold due to the steep behavior of σ .

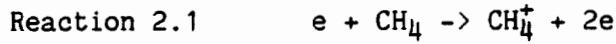
For a number of reactions, the cross sections can also be fit by the formula

$$\sigma = a \left(\frac{E_{th}}{E} \right)^n \ln \left(\frac{E}{E_{th}} \right) ,$$

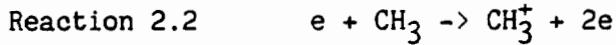
which is an empirical modification of the Bethe-Born formula. The parameters

a and n were evaluated in two ways. We used a least-squares minimization with respect to the parameters with: (1) a uniform weighting, and (2) a weighting ignoring the points at energies below the peak in σ . The first method provides a better match to the entire cross section, but may be inaccurate for the large-E asymptotic dependence. The second method gives a better asymptotic dependence at the expense of a poorer match near the peak. The threshold behavior in the latter case is reasonably accurate because the analytic form of the formula forces it, and this method avoids the problem of the points on the steep part of the curve unduly influencing the least-squares error. Each of these methods works better for different reactions and the tables contain either or both if the match is good. These fits are not as accurate as the polynomial fit, having errors the order of 0.5 to 1, but are smoother. The polynomial fits have oscillatory behavior when their errors are greater than about 10^{-2} . We label the parameters a and n in the Born-like formula by $a_{\text{Born},1}$ and $n_{\text{Born},1}$ for the fits obtained by performing a least-squares fit to all points, and by $a_{\text{Born},2}$ and $n_{\text{Born},2}$ for those obtained with only the points after the peak in σ .

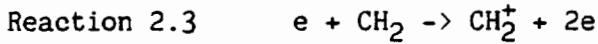
These tables also provide the minimum cross section (σ_{\min} , in cm^2) at the minimum energy (E_{\min} , in eV) for the points considered, and the maximum cross section (σ_{\max} , in cm^2) over the energy range 0.1 eV to 2 keV. In some cases, σ_{\max} may not be the absolute maximum since σ is still increasing for energies either ≥ 2 keV, or ≤ 0.1 eV. Finally, the tables list errors for all of the fits. In general, fits with errors > 0.1 have problems near threshold and should be compared to the curves in the text to determine if they are suitable for a particular calculation. In most of these cases their usefulness depends on the energy range of interest. Fits with errors less than 10^{-2} are nearly indistinguishable from the original curves.



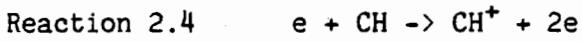
a0 -1.692667783851e+03	a1 2.361715778264e+03	a2 -1.438324660013e+03
a3 4.887024369590e+02	a4 -1.013809397590e+02	a5 1.316222364453e+01
a6 -1.045724814875e+00	a7 4.654403722971e-02	a8 -8.896748338271e-04
E_{min} 1.43e+01	$\sigma(E_{min})$ 1.00e-19	σ_{max} 1.80e-16 Error 2.39e-01



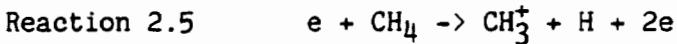
a0 -1.692667783851e+03	a1 2.361715778264e+03	a2 -1.438324660013e+03
a3 4.887024369590e+02	a4 -1.013809397590e+02	a5 1.316222364453e+01
a6 -1.045724814875e+00	a7 4.654403722971e-02	a8 -8.896748338271e-04
E_{min} 1.43e+01	$\sigma(E_{min})$ 1.00e-19	σ_{max} 1.80e-16 Error 2.39e-01



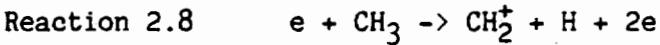
a0 -1.692667783851e+03	a1 2.361715778264e+03	a2 -1.438324660013e+03
a3 4.887024369590e+02	a4 -1.013809397590e+02	a5 1.316222364453e+01
a6 -1.045724814875e+00	a7 4.654403722971e-02	a8 -8.896748338271e-04
E_{min} 1.43e+01	$\sigma(E_{min})$ 1.00e-19	σ_{max} 1.80e-16 Error 2.39e-01



a0 -1.692667783851e+03	a1 2.361715778264e+03	a2 -1.438324660013e+03
a3 4.887024369590e+02	a4 -1.013809397590e+02	a5 1.316222364453e+01
a6 -1.045724814875e+00	a7 4.654403722971e-02	a8 -8.896748338271e-04
E_{min} 1.43e+01	$\sigma(E_{min})$ 1.00e-19	σ_{max} 1.80e-16 Error 2.39e-01



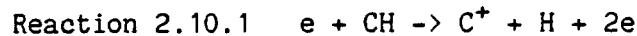
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a3 5.853709727258e+02	a4 -1.201180430705e+02	a5 1.546178211913e+01
a6 -1.220347037545e+00	a7 5.404594929128e-02	a8 -1.029231747694e-03
E_{min} 1.65e+01	$\sigma(E_{min})$ 1.00e-19	σ_{max} 1.36e-16 Error 2.41e-01



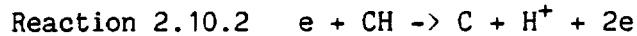
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a3 6.482771887159e+02	a4 -1.340919687035e+02	a5 1.739679380706e+01
a6 -1.383748404263e+00	a7 6.175302055319e-02	a8 -1.184953696321e-03
E_{min} 1.64e+01	$\sigma(E_{min})$ 1.00e-19	σ_{max} 1.04e-16 Error 1.70e-01



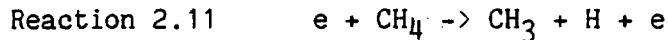
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a3 1.080643868639e+03	a4 -2.241762936520e+02	a5 2.918867976046e+01
a6 -2.331521085084e+00	a7 1.045550093558e-01	a8 -2.017200906749e-03
E_{min} 1.85e+01	$\sigma(E_{min})$ 1.00e-19	σ_{max} 6.55e-17 Error 1.44e-01



a0	-4.219037335054e+03	a1	6.038315450877e+03	a2	-3.742568135459e+03
a3	1.300367872859e+03	a4	-2.771341001674e+02	a5	3.712021463864e+01
a6	-3.053952109089e+00	a7	1.412151190574e-01	a8	-2.812197421847e-03
E_{min}	1.86e+01	$\sigma(E_{min})$	1.00e-19	σ_{max}	3.27e-17
				Error	1.06e-01



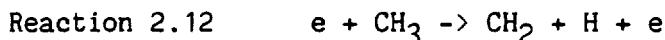
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a3	1.300367872859e+03	a4	-2.771341001674e+02	a5	3.712021463864e+01
a6	-3.053952109089e+00	a7	1.412151190574e-01	a8	-2.812197421847e-03
E_{min}	1.86e+01	$\sigma(E_{min})$	1.00e-19	σ_{max}	3.27e-17
				Error	1.06e-01



a0	-7.056258852633e+02	a1	9.122811970657e+02	a2	-5.244648148915e+02
a3	1.664677700774e+02	a4	-3.196623666735e+01	a5	3.810284445981e+00
a6	-2.759191367117e-01	a7	1.112183198683e-02	a8	-1.914378813397e-04
E_{min}	1.09e+01	$\sigma(E_{min})$	1.00e-19	σ_{max}	2.50e-16
				Error	1.95e-01

aBorn,1= 5.03649e-16 nBorn,1= 7.52472e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 8.98e-01

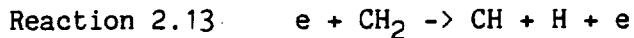
aBorn,2= 5.82458e-16 nBorn,2= 7.99270e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 8.03e-01



a0	-6.839376213284e+02	a1	8.817605905165e+02	a2	-5.066458348962e+02
a3	1.607433982002e+02	a4	-3.085676673287e+01	a5	3.677095278185e+00
a6	-2.662229271054e-01	a7	1.072949220386e-02	a8	-1.846667443936e-04
E_{min}	1.09e+01	$\sigma(E_{min})$	1.00e-19	σ_{max}	1.87e-16
				Error	1.74e-01

aBorn,1= 3.77711e-16 nBorn,1= 7.52448e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 8.50e-01

aBorn,2= 4.36843e-16 nBorn,2= 7.99270e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 7.54e-01



a0 -6.535689559050e+02 a1 8.390361407949e+02 a2 -4.817095803987e+02
a3 1.527347520509e+02 a4 -2.930493284969e+01 a5 3.490839234121e+00
a6 -2.526658330252e-01 a7 1.018101352676e-02 a8 -1.752021947526e-04
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 σ_{max} 1.25e-16 Error 1.47e-01

aBorn,1= 2.51784e-16 nBorn,1= 7.52414e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 7.86e-01

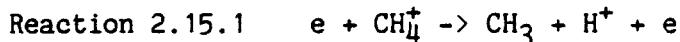
aBorn,2= 2.91229e-16 nBorn,2= 7.99270e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 6.89e-01



a0 -6.022131156964e+02 a1 7.668179739201e+02 a2 -4.395809207748e+02
a3 1.392105575461e+02 a4 -2.668536823803e+01 a5 3.176536664927e+00
a6 -2.297952804076e-01 a7 9.255978330621e-03 a8 -1.592433864624e-04
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 σ_{max} 6.25e-17 Error 1.06e-01

aBorn,1= 1.25872e-16 nBorn,1= 7.52358e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 6.88e-01

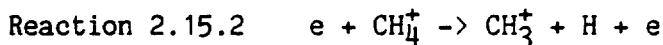
aBorn,2= 1.45614e-16 nBorn,2= 7.99270e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 5.88e-01



a0 -6.022131156964e+02 a1 7.668179739201e+02 a2 -4.395809207748e+02
a3 1.392105575461e+02 a4 -2.668536823803e+01 a5 3.176536664927e+00
a6 -2.297952804076e-01 a7 9.255978330621e-03 a8 -1.592433864624e-04
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 σ_{max} 6.25e-17 Error 1.06e-01

aBorn,1= 1.25872e-16 nBorn,1= 7.52358e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 6.88e-01

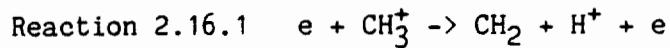
aBorn,2= 1.45614e-16 nBorn,2= 7.99270e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 5.88e-01



a0 -6.839376213284e+02 a1 8.817605905165e+02 a2 -5.066458348962e+02
a3 1.607433982002e+02 a4 -3.085676673287e+01 a5 3.677095278185e+00
a6 -2.662229271054e-01 a7 1.072949220386e-02 a8 -1.846667443936e-04
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 σ_{max} 1.87e-16 Error 1.74e-01

aBorn,1= 3.77711e-16 nBorn,1= 7.52448e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 8.50e-01

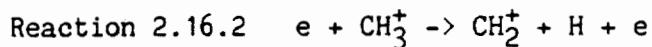
aBorn,2= 4.36843e-16 nBorn,2= 7.99270e-01
E_{min} 1.09e+01 σ(E_{min}) 1.00e-19 Error 7.54e-01



a0 -6.022131156964e+02 a1 7.668179739201e+02 a2 -4.395809207748e+02
a3 1.392105575461e+02 a4 -2.668536823803e+01 a5 3.176536664927e+00
a6 -2.297952804076e-01 a7 9.255978330621e-03 a8 -1.592433864624e-04
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 σ_{max} 6.25e-17 Error 1.06e-01

aBorn,1= 1.25872e-16 nBorn,1= 7.52358e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 6.88e-01

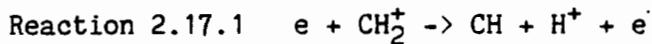
aBorn,2= 1.45614e-16 nBorn,2= 7.99270e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 5.88e-01



a0 -6.535689559050e+02 a1 8.390361407949e+02 a2 -4.817095803987e+02
a3 1.527347520509e+02 a4 -2.930493284969e+01 a5 3.490839234121e+00
a6 -2.526658330252e-01 a7 1.018101352676e-02 a8 -1.752021947526e-04
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 σ_{max} 1.25e-16 Error 1.47e-01

aBorn,1= 2.51784e-16 nBorn,1= 7.52414e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 7.86e-01

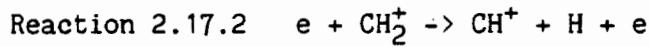
aBorn,2= 2.91229e-16 nBorn,2= 7.99270e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 6.89e-01



a0 -6.022131156964e+02 a1 7.668179739201e+02 a2 -4.395809207748e+02
a3 1.392105575461e+02 a4 -2.668536823803e+01 a5 3.176536664927e+00
a6 -2.297952804076e-01 a7 9.255978330621e-03 a8 -1.592433864624e-04
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 σ_{max} 6.25e-17 Error 1.06e-01

aBorn,1= 1.25872e-16 nBorn,1= 7.52358e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 6.88e-01

aBorn,2= 1.45614e-16 nBorn,2= 7.99270e-01
 E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 5.88e-01

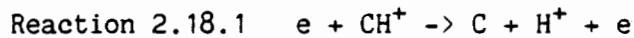


a0	-6.022131156964e+02	a1	7.668179739201e+02	a2	-4.395809207748e+02
a3	1.392105575461e+02	a4	-2.668536823803e+01	a5	3.176536664927e+00
a6	-2.297952804076e-01	a7	9.255978330621e-03	a8	-1.592433864624e-04
E _{min}	1.09e+01	$\sigma(E_{min})$	1.00e-19	σ_{max}	6.25e-17

Error 1.06e-01

aBorn,1= 1.25872e-16 nBorn,1= 7.52358e-01
E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 6.88e-01

aBorn,2= 1.45614e-16 nBorn,2= 7.99270e-01
E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 5.88e-01



a0	-5.515975857720e+02	a1	6.956832993419e+02	a2	-3.981129480710e+02
a3	1.259064376679e+02	a4	-2.410977200352e+01	a5	2.867649348478e+00
a6	-2.073276391269e-01	a7	8.347553168754e-03	a8	-1.435758909644e-04
E _{min}	1.09e+01	$\sigma(E_{min})$	1.00e-19	σ_{max}	3.12e-17

Error 7.25e-02

aBorn,1= 6.29278e-17 nBorn,1= 7.52310e-01
E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 6.03e-01

aBorn,2= 7.28072e-17 nBorn,2= 7.99270e-01
E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 5.00e-01



a0	-5.515975857720e+02	a1	6.956832993419e+02	a2	-3.981129480710e+02
a3	1.259064376679e+02	a4	-2.410977200352e+01	a5	2.867649348478e+00
a6	-2.073276391269e-01	a7	8.347553168754e-03	a8	-1.435758909644e-04
E _{min}	1.09e+01	$\sigma(E_{min})$	1.00e-19	σ_{max}	3.12e-17

Error 7.25e-02

aBorn,1= 6.29278e-17 nBorn,1= 7.52310e-01
E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 6.03e-01

aBorn,2= 7.28072e-17 nBorn,2= 7.99270e-01
E_{min} 1.09e+01 $\sigma(E_{min})$ 1.00e-19 Error 5.00e-01



a0	-3.661792759246e+01	a1	-1.599538793409e+00	a2	-1.337709595139e-03
a3	-2.149485975053e-04	a4	8.803347518288e-04	a5	-1.605640463871e-04
a6	-1.272130426378e-04	a7	4.972542282664e-05	a8	-4.902344178631e-06
E _{min}	1.00e-01	$\sigma(E_{min})$	4.92e-15	σ_{max}	4.92e-15

Error 1.80e-07



a0 -3.551946244714e+01	a1 -1.599104551548e+00	a2 -8.117117322324e-04
a3 -7.59375888596e-04	a4 6.551910669416e-04	a5 2.912393605786e-05
a6 -1.162856460123e-04	a7 2.959455203689e-05	a8 -2.266280687412e-06
E _{min} 1.00e-01	σ(E _{min}) 1.48e-14	σ _{max} 1.48e-14 Error 2.16e-07



a0 -3.489627799928e+01	a1 -1.490828612573e+00	a2 -7.757347328285e-04
a3 -8.642967106244e-03	a4 3.096055948101e-03	a5 1.168191487324e-03
a6 -7.941869052814e-04	a7 1.444325051687e-04	a8 -8.721644817513e-06
E _{min} 1.00e-01	σ(E _{min}) 2.00e-14	σ _{max} 2.00e-14 Error 2.05e-05



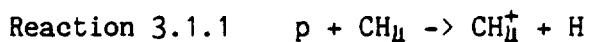
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a3 4.273275442080e-02	a4 7.800843662937e-02	a5 -1.869971551862e-02
a6 -5.167329673693e-03	a7 2.167238257016e-03	a8 -1.939809654826e-04
E _{min} 1.00e-01	σ(E _{min}) 1.70e-14	σ _{max} 1.70e-14 Error 5.89e-04



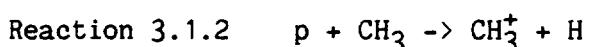
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a3 4.732298607515e-02	a4 7.998743710929e-02	a5 -2.029356025352e-02
a6 -5.271985502076e-03	a7 2.336428791132e-03	a8 -2.156372558830e-04
E _{min} 1.00e-01	σ(E _{min}) 1.20e-14	σ _{max} 1.20e-14 Error 5.80e-04



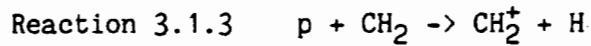
a0 -7.661645944850e+02	a1 9.615002727652e+02	a2 -5.375226827033e+02
a3 1.667633808971e+02	a4 -3.141510479736e+01	a5 3.682673653813e+00
a6 -2.627307121325e-01	a7 1.044757315189e-02	a8 -1.776120342550e-04
E _{min} 1.25e+01	σ(E _{min}) 1.00e-19	σ _{max} 4.20e-16 Error 1.52e-01



a0 -3.327850106693e+01	a1 -1.608383489195e-01	a2 1.886899005822e-01
a3 -4.166534111130e-02	a4 -1.210872012273e-02	a5 6.257737886111e-03
a6 -9.723353373635e-04	a7 6.518598900821e-05	a8 -1.618150392864e-06
E _{min} 1.00e-01	σ(E _{min}) 1.01e-14	σ _{max} 1.01e-14 Error 9.87e-03



a0 -3.327850106693e+01	a1 -1.608383489195e-01	a2 1.886899005822e-01
a3 -4.166534111130e-02	a4 -1.210872012273e-02	a5 6.257737886111e-03
a6 -9.723353373635e-04	a7 6.518598900821e-05	a8 -1.618150392864e-06
E _{min} 1.00e-01	σ(E _{min}) 1.01e-14	σ _{max} 1.01e-14 Error 9.87e-03



a0 -3.327850106693e+01	a1 -1.608383489195e-01	a2 1.886899005822e-01
a3 -4.166534111130e-02	a4 -1.210872012273e-02	a5 6.257737886111e-03
a6 -9.723353373635e-04	a7 6.518598900821e-05	a8 -1.618150392864e-06
E _{min} 1.00e-01	σ(E _{min}) 1.01e-14	σ _{max} 1.01e-14 Error 9.87e-03



a0 -3.327850106693e+01	a1 -1.608383489195e-01	a2 1.886899005822e-01
a3 -4.166534111130e-02	a4 -1.210872012273e-02	a5 6.257737886111e-03
a6 -9.723353373635e-04	a7 6.518598900821e-05	a8 -1.618150392864e-06
E _{min} 1.00e-01	σ(E _{min}) 1.01e-14	σ _{max} 1.01e-14 Error 9.87e-03



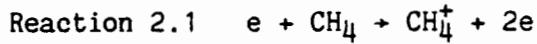
a0 -7.465460177166e+01	a1 2.248859715942e+01	a2 1.636561439622e+00
a3 -4.518322900175e+00	a4 1.485788398238e+00	a5 -2.286969609061e-01
a6 1.860340466289e-02	a7 -7.698589606030e-04	a8 1.270828631381e-05
E _{min} 5.75e+00	σ(E _{min}) 1.00e-19	σ _{max} 6.77e-16 Error 1.29e-02

4.2 Polynomial Fits for $\langle\sigma v\rangle$ for Electron Reactions

We present nine-term polynomial fits for $\langle\sigma v\rangle$ for the electron reactions with the following formula

$$\ln \langle\sigma v\rangle = \sum_{n=0}^8 b_n (\ln T)^n .$$

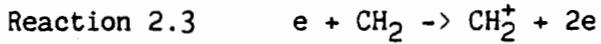
For these reactions, the energy of the target particle can be considered to be zero. For all of the fits, we list the coefficients b_n , the errors, the minimum temperature T_{\min} that was fit, $\langle\sigma v\rangle$ at the minimum temperature, and the maximum $\langle\sigma v\rangle$ over the temperature range 0.1 eV to 2 keV. In all cases, the errors are small, and the fits cannot be distinguished from the data on a plot of the kind used for the figures in the text.



b0 -3.130271609338e+01	b1 1.296168986190e+01	b2 -5.500277167544e+00
b3 1.468759127748e+00	b4 -2.515405069844e-01	b5 2.710024229192e-02
b6 -1.786606299569e-03	b7 6.605572407734e-05	b8 -1.051047534357e-06
T_{min} 1.58e+00	$\langle\sigma v\rangle(T_{min})$ 3.52e-12	$\langle\sigma v\rangle_{max}$ 1.04e-07 Error 3.54e-06



b0 -3.130271609338e+01	b1 1.296168986190e+01	b2 -5.500277167544e+00
b3 1.468759127748e+00	b4 -2.515405069844e-01	b5 2.710024229192e-02
b6 -1.786606299569e-03	b7 6.605572407734e-05	b8 -1.051047534357e-06
T_{min} 1.58e+00	$\langle\sigma v\rangle(T_{min})$ 3.52e-12	$\langle\sigma v\rangle_{max}$ 1.04e-07 Error 3.54e-06



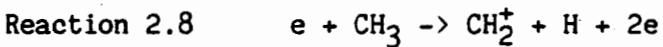
b0 -3.130271609338e+01	b1 1.296168986190e+01	b2 -5.500277167544e+00
b3 1.468759127748e+00	b4 -2.515405069844e-01	b5 2.710024229192e-02
b6 -1.786606299569e-03	b7 6.605572407734e-05	b8 -1.051047534357e-06
T_{min} 1.58e+00	$\langle\sigma v\rangle(T_{min})$ 3.52e-12	$\langle\sigma v\rangle_{max}$ 1.04e-07 Error 3.54e-06



b0 -3.130271609338e+01	b1 1.296168986190e+01	b2 -5.500277167544e+00
b3 1.468759127748e+00	b4 -2.515405069844e-01	b5 2.710024229192e-02
b6 -1.786606299569e-03	b7 6.605572407734e-05	b8 -1.051047534357e-06
T_{min} 1.58e+00	$\langle\sigma v\rangle(T_{min})$ 3.52e-12	$\langle\sigma v\rangle_{max}$ 1.04e-07 Error 3.54e-06



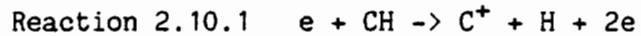
b0 -3.306634718031e+01	b1 1.416521389189e+01	b2 -5.811967385794e+00
b3 1.470177820879e+00	b4 -2.390021646165e-01	b5 2.491401203694e-02
b6 -1.636717239458e-03	b7 6.236047157828e-05	b8 -1.054699569134e-06
T_{min} 2.00e+00	$\langle\sigma v\rangle(T_{min})$ 7.39e-12	$\langle\sigma v\rangle_{max}$ 7.67e-08 Error 3.07e-05



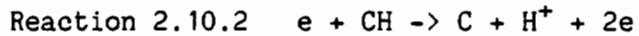
b0 -3.388016314847e+01	b1 1.465034994470e+01	b2 -6.016241495970e+00
b3 1.516215017478e+00	b4 -2.428453509838e-01	b5 2.456763798440e-02
b6 -1.540625099005e-03	b7 5.523892168286e-05	b8 -8.715463490510e-07
T_{min} 2.00e+00	$\langle\sigma v\rangle(T_{min})$ 4.24e-12	$\langle\sigma v\rangle_{max}$ 6.33e-08 Error 2.84e-06



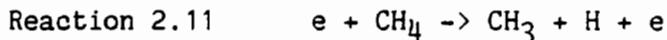
b0 -3.611375048015e+01	b1 1.702018604424e+01	b2 -7.450989420377e+00
b3 2.011285031949e+00	b4 -3.461964892218e-01	b5 3.776562998994e-02
b6 -2.546859178541e-03	b7 9.730219545464e-05	b8 -1.613604371753e-06
T_{min} 2.51e+00	$\langle\sigma v\rangle(T_{min})$ 9.21e-12	$\langle\sigma v\rangle_{max}$ 4.03e-08 Error 3.91e-06



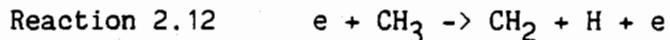
b0	-3.680913942497e+01	b1	1.702452241875e+01	b2	-7.454313548061e+00
b3	2.012620972667e+00	b4	-3.465080963663e-01	b5	3.780928049163e-02
b6	-2.550477120094e-03	b7	9.746560933107e-05	b8	-1.616702702130e-06
T_{min}	2.51e+00	$\langle\sigma v\rangle(T_{min})$	4.60e-12	$\langle\sigma v\rangle_{max}$	2.01e-08 Error 3.89e-06



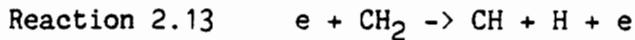
b0	-3.680913942497e+01	b1	1.702452241875e+01	b2	-7.454313548061e+00
b3	2.012620972667e+00	b4	-3.465080963663e-01	b5	3.780928049163e-02
b6	-2.550477120094e-03	b7	9.746560933107e-05	b8	-1.616702702130e-06
T_{min}	2.51e+00	$\langle\sigma v\rangle(T_{min})$	4.60e-12	$\langle\sigma v\rangle_{max}$	2.01e-08 Error 3.89e-06



b0	-2.807275946645e+01	b1	1.108212341826e+01	b2	-4.959611559863e+00
b3	1.392349178986e+00	b4	-2.573267587051e-01	b5	3.121418393954e-02
b6	-2.395406694410e-03	b7	1.050840706958e-04	b8	-1.996822469861e-06
T_{min}	1.26e+00	$\langle\sigma v\rangle(T_{min})$	6.42e-12	$\langle\sigma v\rangle_{max}$	1.31e-07 Error 1.49e-05



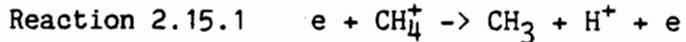
b0	-2.836044146959e+01	b1	1.108212347679e+01	b2	-4.959611754095e+00
b3	1.392349312989e+00	b4	-2.573268016867e-01	b5	3.121419141368e-02
b6	-2.395407419896e-03	b7	1.050841076770e-04	b8	-1.996823241480e-06
T_{min}	1.26e+00	$\langle\sigma v\rangle(T_{min})$	4.82e-12	$\langle\sigma v\rangle_{max}$	9.84e-08 Error 1.49e-05



b0	-2.876590642619e+01	b1	1.108212244292e+01	b2	-4.959610449105e+00
b3	1.392348609760e+00	b4	-2.573266019767e-01	b5	3.121415917105e-02
b6	-2.395404444673e-03	b7	1.050839615167e-04	b8	-1.996820276763e-06
T_{min}	1.26e+00	$\langle\sigma v\rangle(T_{min})$	3.21e-12	$\langle\sigma v\rangle_{max}$	6.56e-08 Error 1.49e-05



b0	-2.945957131327e+01	b1	1.108352512038e+01	b2	-4.960967637555e+00
b3	1.392993579033e+00	b4	-2.574970898281e-01	b5	3.124045642701e-02
b6	-2.397756481445e-03	b7	1.051969352717e-04	b8	-1.999073436426e-06
T_{min}	1.26e+00	$\langle\sigma v\rangle(T_{min})$	1.60e-12	$\langle\sigma v\rangle_{max}$	3.28e-08 Error 1.50e-05



b0	-2.945957131327e+01	b1	1.108352512038e+01	b2	-4.960967637555e+00
b3	1.392993579033e+00	b4	-2.574970898281e-01	b5	3.124045642701e-02
b6	-2.397756481445e-03	b7	1.051969352717e-04	b8	-1.999073436426e-06
T_{min}	1.26e+00	$\langle\sigma v\rangle(T_{min})$	1.60e-12	$\langle\sigma v\rangle_{max}$	3.28e-08 Error 1.50e-05

Reaction 2.15.2 e + CH ₄ ⁺ → CH ₃ ⁺ + H + e							
b0 -2.836044146959e+01	b1 1.108212347679e+01	b2 -4.959611754095e+00					
b3 1.392349312989e+00	b4 -2.573268016867e-01	b5 3.121419141368e-02					
b6 -2.395407419896e-03	b7 1.050841076770e-04	b8 -1.996823241480e-06					
T _{min} 1.26e+00	<σv>(T _{min}) 4.82e-12	<σv> _{max} 9.84e-08	Error 1.49e-05				
Reaction 2.16.1 e + CH ₃ ⁺ → CH ₂ ⁺ + H ⁺ + e							
b0 -2.945957131327e+01	b1 1.108352512038e+01	b2 -4.960967637555e+00					
b3 1.392993579033e+00	b4 -2.574970898281e-01	b5 3.124045642701e-02					
b6 -2.397756481445e-03	b7 1.051969352717e-04	b8 -1.999073436426e-06					
T _{min} 1.26e+00	<σv>(T _{min}) 1.60e-12	<σv> _{max} 3.28e-08	Error 1.50e-05				
Reaction 2.16.2 e + CH ₂ ⁺ → CH ₃ ⁺ + H + e							
b0 -2.876590642619e+01	b1 1.108212244292e+01	b2 -4.959610449105e+00					
b3 1.392348609760e+00	b4 -2.573266019767e-01	b5 3.121415917105e-02					
b6 -2.39540444673e-03	b7 1.050839615167e-04	b8 -1.996820276763e-06					
T _{min} 1.26e+00	<σv>(T _{min}) 3.21e-12	<σv> _{max} 6.56e-08	Error 1.49e-05				
Reaction 2.17.1 e + CH ₂ ⁺ → CH + H ⁺ + e							
b0 -2.945957131327e+01	b1 1.108352512038e+01	b2 -4.960967637555e+00					
b3 1.392993579033e+00	b4 -2.574970898281e-01	b5 3.124045642701e-02					
b6 -2.397756481445e-03	b7 1.051969352717e-04	b8 -1.999073436426e-06					
T _{min} 1.26e+00	<σv>(T _{min}) 1.60e-12	<σv> _{max} 3.28e-08	Error 1.50e-05				
Reaction 2.17.2 e + CH ₂ ⁺ → CH ⁺ + H + e							
b0 -2.945957131327e+01	b1 1.108352512038e+01	b2 -4.960967637555e+00					
b3 1.392993579033e+00	b4 -2.574970898281e-01	b5 3.124045642701e-02					
b6 -2.397756481445e-03	b7 1.051969352717e-04	b8 -1.999073436426e-06					
T _{min} 1.26e+00	<σv>(T _{min}) 1.60e-12	<σv> _{max} 3.28e-08	Error 1.50e-05				
Reaction 2.18.1 e + CH ⁺ → C + H ⁺ + e							
b0 -3.012032364373e+01	b1 1.099522112261e+01	b2 -4.875231901753e+00					
b3 1.352160807859e+00	b4 -2.466874895760e-01	b5 2.957131757726e-02					
b6 -2.248347614716e-03	b7 9.801598372843e-05	b8 -1.855784198949e-06					
T _{min} 1.58e+00	<σv>(T _{min}) 5.25e-12	<σv> _{max} 1.64e-08	Error 1.37e-05				
Reaction 2.18.2 e + CH ⁺ → C ⁺ + H + e							
b0 -3.012032364373e+01	b1 1.099522112261e+01	b2 -4.875231901753e+00					
b3 1.352160807859e+00	b4 -2.466874895760e-01	b5 2.957131757726e-02					
b6 -2.248347614716e-03	b7 9.801598372843e-05	b8 -1.855784198949e-06					
T _{min} 1.58e+00	<σv>(T _{min}) 5.25e-12	<σv> _{max} 1.64e-08	Error 1.37e-05				

Reaction 2.19.1	$e + \text{CH}_4^+ \rightarrow \text{CH}_3 + \text{H}$		
b0	-1.811008536904e+01	b1	-9.609633964487e-01
b3	6.125083185220e-03	b4	-7.398087967535e-04
b6	1.489613542998e-05	b7	-2.305875698910e-06
T _{min}	1.00e-01	<σv>(T _{min})	9.47e-08 <σv> _{max} 9.47e-08 Error 2.32e-09
b2	-3.424995112490e-02	b5	1.023424811982e-05
b8	1.121715693015e-07		
Reaction 2.19.2	$e + \text{CH}_4^+ \rightarrow \text{CH}_2 + 2\text{H}$		
b0	-1.701143581095e+01	b1	-9.608594282939e-01
b3	6.062830823689e-03	b4	-6.960604032613e-04
b6	9.608674057752e-06	b7	-1.294529653721e-06
T _{min}	1.00e-01	<σv>(T _{min})	2.84e-07 <σv> _{max} 2.84e-07 Error 5.51e-09
b2	-3.434403515564e-02	b5	1.300409033176e-05
b8	5.355898675023e-08		
Reaction 2.20	$e + \text{CH}_3^+ \rightarrow \text{CH}_2 + \text{H}$		
b0	-1.651879578335e+01	b1	-8.845965948845e-01
b3	5.931429828017e-03	b4	-6.065683500746e-04
b6	1.013117512304e-05	b7	-1.075059322040e-06
T _{min}	1.00e-01	<σv>(T _{min})	3.97e-07 <σv> _{max} 3.97e-07 Error 1.79e-08
b2	-3.234169762966e-02	b5	-6.807256725287e-06
b8	3.738529146504e-08		
Reaction 2.21	$e + \text{CH}_2^+ \rightarrow \text{CH} + \text{H}$		
b0	-1.615383183840e+01	b1	-7.586474440302e-01
b3	-6.965630710151e-04	b4	4.528628288339e-03
b6	-1.975435184873e-05	b7	1.058151325615e-05
T _{min}	1.00e-01	<σv>(T _{min})	3.60e-07 <σv> _{max} 3.60e-07 Error 2.03e-06
b2	-1.130528453633e-01	b5	-6.557967171201e-04
b8	-6.041276398828e-07		
Reaction 2.22	$e + \text{CH}^+ \rightarrow \text{C} + \text{H}$		
b0	-1.650186471548e+01	b1	-7.577994435524e-01
b3	-1.208054036514e-03	b4	4.852655512390e-03
b6	-5.978237115279e-05	b7	1.788694174879e-05
T _{min}	1.00e-01	<σv>(T _{min})	2.54e-07 <σv> _{max} 2.54e-07 Error 1.56e-06
b2	-1.137373258287e-01	b5	-6.277507371151e-04
b8	-1.012452989015e-06		
Reaction 2.23	$e + \text{C} \rightarrow \text{C}^+ + 2\text{e}$		
b0	-3.003325031029e+01	b1	1.210620585621e+01
b3	1.191377262469e+00	b4	-1.959147085306e-01
b6	-1.323291115275e-03	b7	4.667595732505e-05
T _{min}	1.58e+00	<σv>(T _{min})	9.64e-12 <σv> _{max} 1.97e-07 Error 9.04e-07
b2	-4.784495376444e+00	b5	2.063978055880e-02
b8	-6.915444216285e-07		

4.3 Double Polynomial Fits for $\langle\sigma v\rangle$

For reactions between two heavy particles, one often needs the reaction rate coefficients as a function of both the temperature T of the plasma particles and the energy E of the incident particle. We have made such fits by constructing nine by nine term polynomial fits for $\ln \langle\sigma v\rangle$ in terms of $\ln E$ and $\ln T$ in the form

$$\ln \langle\sigma v\rangle = \sum_{i=0}^8 \sum_{j=0}^8 a_{ij} (\ln E)^i (\ln T)^j ,$$

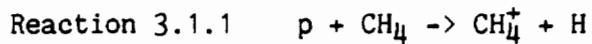
and list the coefficients a_{ij} in the tables.

These fits should be used with some care. They are valid for the range $0.1 \text{ eV} < E < 2 \text{ keV}$ and $0.1 \text{ eV} < T < 2 \text{ keV}$ provided $\langle\sigma v\rangle$ is greater than $10^{-11} \text{ cm}^3/\text{s}$. We made no attempt to fit very low values of $\langle\sigma v\rangle$ since this tends to reduce the accuracy of the fit at larger values. Since no attempt was made to fit these low values, it is possible that the fit may give high (incorrect) values of $\langle\sigma v\rangle$ outside the range of E and T for which $\langle\sigma v\rangle$ is greater than $10^{-11} \text{ cm}^3/\text{s}$. In using these tables, the reader should be aware that, if the fit gives a value of $\langle\sigma v\rangle$ greater than $10^{-11} \text{ cm}^3/\text{s}$, it is not a sufficient condition for the fit to be accurate. It must be checked that E and T are in the range for which $\langle\sigma v\rangle$ is truly greater than cm^3/s .

The tables provide an error for each fit which is the average root-mean-square error in the fit, relative to the maximum, $\langle\sigma v\rangle_{\max}$, of $\langle\sigma v\rangle$ in the entire E, T range. The error is given by

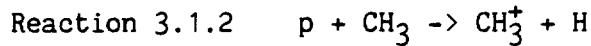
$$\text{Error} = \frac{1}{N\langle\sigma v\rangle_{\max}} \left[\sum_{ij} \left(\langle\sigma v\rangle_{ij} - \langle\sigma v\rangle_{ij}^{\text{fit}} \right)^2 \right]^{1/2} ;$$

where $\langle \sigma v \rangle_{ij}$ and $\langle \sigma v \rangle_{ij}^{fit}$ are values of the calculated and the fit $\langle \sigma v \rangle$'s respectively, at the points E_i and T_j , and N is the number of values included in the sum. Only terms with $\langle \sigma v \rangle$ greater than $10^{-11} \text{ cm}^3/\text{s}$ are included in the sum.



	E Index	0	1	2
T Index				
0	-1.893309642087e+01	1.630850139987e-02	-4.714272469978e-03	
1	3.776884529381e-01	1.048145245940e-02	7.227733247236e-05	
2	1.093763179118e-01	-8.946299454637e-03	5.444574390551e-05	
3	-2.977414700946e-02	6.502084407985e-04	1.092361098382e-03	
4	-3.266919857975e-03	5.754254352327e-04	-4.134810722987e-04	
5	2.833761994929e-03	-1.586203199222e-04	2.109974461716e-05	
6	-4.972454353280e-04	1.695706232098e-05	8.410801850446e-06	
7	3.578860489665e-05	-8.046520550513e-07	-1.200952674126e-06	
8	-9.350695669585e-07	1.323413496981e-08	4.527497936811e-08	
	E Index	3	4	5
T Index				
0	2.425492370093e-03	3.068101950239e-03	-1.633878600590e-04	
1	-7.529649417774e-03	-2.850523369529e-04	6.156392408384e-04	
2	1.707309355637e-03	-4.053883564956e-04	-9.550753935009e-05	
3	3.818918718530e-04	-6.507215186222e-05	-2.145885656470e-05	
4	-1.147415418920e-04	7.428734189103e-05	-4.614052740801e-06	
5	2.696892676495e-06	-1.176543808697e-05	2.542597558870e-06	
6	1.009068906397e-06	2.076254405295e-07	-2.044216076319e-07	
7	-6.821482596551e-08	7.011617376997e-08	-4.372775978657e-09	
8	7.145677893147e-10	-3.693880360696e-09	6.489051753343e-10	
	E Index	6	7	8
T Index				
0	-1.023569804176e-04	1.421483822630e-05	-5.300227927218e-07	
1	-1.035125430666e-04	6.780400601184e-06	-1.596091897574e-07	
2	3.495664394328e-05	-3.364738102350e-06	1.057092818237e-07	
3	4.842220252995e-06	-3.124588766143e-07	6.085162418331e-09	
4	-1.313512598842e-06	1.834508345923e-07	-6.495489280153e-09	
5	-7.794570475980e-08	-1.593741872383e-08	9.506440609074e-10	
6	1.818970018754e-08	6.647545290109e-10	-8.054668689989e-11	
7	1.989805345252e-10	-8.636301826823e-11	5.648949950364e-12	
8	-6.425242445187e-11	5.232989348622e-12	-2.053898151891e-13	

Error 4.76e-04



E Index	0	1	2
T Index			
0	-1.893015025400e+01	1.389143067153e-02	-6.781236636920e-03
1	3.779899373076e-01	1.026502385650e-02	-7.698088894683e-04
2	1.089496905822e-01	-9.157490505951e-03	2.969884378880e-04
3	-2.975011439547e-02	8.301595755376e-04	1.176745452526e-03
4	-3.248776015585e-03	5.779936403988e-04	-4.344370519201e-04
5	2.830654621739e-03	-1.747494577437e-04	1.958192848998e-05
6	-4.971444551136e-04	2.030387364220e-05	9.119763233765e-06
7	3.579805599493e-05	-1.073274942848e-06	-1.262470635022e-06
8	-9.356043099030e-07	2.095831478302e-08	4.696957441923e-08
E Index	3	4	5
T Index			
0	4.708492665561e-03	3.222294058983e-03	-4.354492180290e-04
1	-7.715282476671e-03	-1.893334421394e-04	6.225946617245e-04
2	1.668665562961e-03	-4.418488177370e-04	-8.252345657352e-05
3	3.570817130729e-04	-7.121562671774e-05	-1.995855695331e-05
4	-1.118613768332e-04	7.742141754581e-05	-5.506766569456e-06
5	5.038579776254e-06	-1.212485117935e-05	2.573708762225e-06
6	4.127343809761e-07	2.242442284292e-07	-1.896502386406e-07
7	-1.677674612550e-08	6.952443112677e-08	-6.036487436644e-09
8	-8.131627877359e-10	-3.668215799893e-09	6.997898343755e-10
E Index	6	7	8
T Index			
0	-4.825375453335e-05	9.977523040655e-06	-4.110277889686e-07
1	-1.082000663592e-04	7.268416351651e-06	-1.753527041780e-07
2	3.335975599670e-05	-3.282019035422e-06	1.042369042400e-07
3	4.851555584220e-06	-3.281444793300e-07	6.823060985962e-09
4	-1.238095500910e-06	1.822869211146e-07	-6.562368829665e-09
5	-8.352452578849e-08	-1.532146244890e-08	9.290573255333e-10
6	1.719741056841e-08	5.973202009088e-10	-7.531799873037e-11
7	3.408657452954e-10	-8.362107501242e-11	5.246746788544e-12
8	-6.905194380153e-11	5.201295647464e-12	-1.947010286302e-13

Error 4.91e-04

Reaction 3.1.3 p + CH₂ → CH₂⁺ + H

T Index	E Index	0	1	2
0	-1.892741490024e+01	1.152420986793e-02	-8.780888101054e-03	
1	3.788098456684e-01	9.000972529774e-03	-1.876509952765e-03	
2	1.090725061232e-01	-9.695960467242e-03	3.111706544768e-04	
3	-3.000449680436e-02	1.485532220237e-03	1.296841607829e-03	
4	-3.279542407570e-03	5.652830426608e-04	-4.203504358609e-04	
5	2.865807364045e-03	-2.405403814714e-04	1.313418239934e-05	
6	-5.035888740641e-04	3.590614373961e-05	8.783410077194e-06	
7	3.626463829777e-05	-2.452619126791e-06	-1.106391575461e-06	
8	-9.475996387093e-07	6.404591761204e-08	3.871143936175e-08	
T Index	E Index	3	4	5
0	7.182298047960e-03	3.357963007674e-03	-7.270848383381e-04	
1	-7.660318957536e-03	-8.703197824891e-05	6.084573282880e-04	
2	1.683720541775e-03	-4.531927064772e-04	-7.859006453761e-05	
3	2.498887361524e-04	-7.270758931961e-05	-1.376436553543e-05	
4	-1.079342884921e-04	7.556045192812e-05	-5.321560049855e-06	
5	1.451569314628e-05	-1.264521083892e-05	2.224266459969e-06	
6	-1.669615482481e-06	5.659788755108e-07	-1.750602933349e-07	
7	1.489259906003e-07	2.449872435024e-08	-2.024691997811e-09	
8	-5.407280151576e-09	-1.865823448547e-09	4.236089219820e-10	
T Index	E Index	6	7	8
0	1.091981451234e-05	5.291983408387e-06	-2.784485237271e-07	
1	-1.087411664036e-04	7.436649225082e-06	-1.821937118550e-07	
2	3.281188936769e-05	-3.249845228521e-06	1.035835180270e-07	
3	3.861915548886e-06	-2.675185753286e-07	5.504045770260e-09	
4	-1.242543887401e-06	1.823296753458e-07	-6.572917931547e-09	
5	-2.170386158459e-08	-1.910235275312e-08	1.007926779341e-09	
6	1.111261631954e-08	9.817255419496e-10	-8.193222019769e-11	
7	1.746373535520e-10	-7.478956586819e-11	4.831022711092e-12	
8	-4.326898079558e-11	3.656578646932e-12	-1.519531987892e-13	

Error 5.11e-04

Reaction 3.1.4 p + CH → CH⁺ + H

	E Index	0	1	2
T Index				
0	-1.892389432736e+01	8.886284345584e-03	-1.109300880346e-02	
1	3.791545123515e-01	8.475134434604e-03	-2.973010109645e-03	
2	1.085777338734e-01	-9.990530830098e-03	6.446889461501e-04	
3	-2.997534308810e-02	1.713544431587e-03	1.373586207056e-03	
4	-3.260996214109e-03	5.763633536150e-04	-4.480196094509e-04	
5	2.863922977162e-03	-2.617206664923e-04	1.438290421753e-05	
6	-5.038991956580e-04	3.992826597099e-05	9.107700403461e-06	
7	3.631854565763e-05	-2.755740015697e-06	-1.146833082454e-06	
8	-9.497184774037e-07	7.230406803998e-08	4.006171386613e-08	
	E Index	3	4	5
T Index				
0	9.891958133741e-03	3.522032366810e-03	-1.049400447938e-03	
1	-7.781044625266e-03	3.464768381132e-05	6.045693040532e-04	
2	1.634731775121e-03	-5.010651980603e-04	-6.225015839420e-05	
3	2.215628364409e-04	-7.914800428968e-05	-1.192386073197e-05	
4	-1.054043956245e-04	7.984411714572e-05	-6.435098464842e-06	
5	1.697295195994e-05	-1.324570737982e-05	2.296164298139e-06	
6	-2.255156800466e-06	5.933171429767e-07	-1.616686267082e-07	
7	1.977586178919e-07	2.504023290886e-08	-4.009927544303e-09	
8	-6.828266134182e-09	-1.922660210612e-09	4.965121146332e-10	
	E Index	6	7	8
T Index				
0	7.576825283904e-05	1.828073909406e-07	-1.344276753890e-07	
1	-1.118911888932e-04	7.823262706391e-06	-1.953022685282e-07	
2	3.093317830888e-05	-3.165066380853e-06	1.025231510021e-07	
3	3.821918256505e-06	-2.803647165215e-07	6.180674471800e-09	
4	-1.163155113152e-06	1.828672477268e-07	-6.733895111826e-09	
5	-2.867987544661e-08	-1.865893333810e-08	9.972303921835e-10	
6	1.025765387662e-08	9.006547570731e-10	-7.616327775842e-11	
7	3.376813463046e-10	-7.111784442785e-11	4.338865744046e-12	
8	-5.003679679618e-11	3.658641743778e-12	-1.394548455624e-13	

Error 5.58e-04

Reaction 3.2 $p + C \rightarrow C^+ + H$

E Index	0	1	2
T Index			
0	-5.443659700109e+01	4.073411220060e+00	1.343537080718e+00
1	3.519668118251e+01	-7.442349347208e+00	-1.679246081597e+00
2	-1.440577315368e+01	4.967811697956e+00	3.770572537247e-01
3	2.389215208509e+00	-1.609634901952e+00	1.813516675472e-01
4	4.009158278020e-02	2.721115624720e-01	-1.057427190049e-01
5	-6.925835962750e-02	-2.269114466358e-02	2.167917859821e-02
6	9.718717487684e-03	5.787459308821e-04	-2.219154740081e-03
7	-5.743071740355e-04	3.197508385415e-05	1.138421156169e-04
8	1.283086677986e-05	-1.673461633606e-06	-2.333743575530e-06
E Index	3	4	5
T Index			
0	-3.742953182096e-01	1.562786664968e-01	-5.050566764114e-02
1	8.354823234939e-01	-2.057568648831e-01	3.971780176781e-02
2	-4.826530418539e-01	1.210673763876e-01	-1.728640079568e-02
3	9.844891930043e-02	-3.512672315597e-02	4.843632501303e-03
4	1.991164735704e-03	4.344502662194e-03	-7.697368486675e-04
5	-3.840068723237e-03	4.523377512297e-05	4.856982614492e-05
6	6.052986380212e-04	-6.560347179004e-05	2.224934908993e-06
7	-3.961495494005e-05	5.987253800332e-06	-4.426701306196e-07
8	9.679360311336e-07	-1.731952061869e-07	1.580906137037e-08
E Index	6	7	8
T Index			
0	7.600393480264e-03	-5.219982007449e-04	1.343520388572e-05
1	-4.808567649579e-03	3.000417510833e-04	-7.344906981331e-06
2	1.539570238715e-03	-7.810375205427e-05	1.691291158136e-06
3	-3.320115825286e-04	1.084787340601e-05	-1.243722459881e-07
4	5.109863768673e-05	-1.095330615678e-06	-7.965630839833e-09
5	-4.687932503830e-06	1.337796016066e-07	9.339085034104e-11
6	1.375628810844e-07	-1.328023738582e-08	2.989117828849e-10
7	9.667766366726e-09	6.171653468413e-10	-2.961480504137e-11
8	-5.791521078290e-10	-8.319090984891e-12	8.282715522960e-13

Error 8.02e-03

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